



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:16 AM UTC

PDB ID : 1LIK / pdb_00001lik
Title : STRUCTURE OF T. GONDII ADENOSINE KINASE BOUND TO ADENOSINE
Authors : Schumacher, M.A.; Scott, D.M.; Mathews, I.I.; Ealick, S.E.; Roos, D.S.; Ullman, B.; Brennan, R.G.
Deposited on : 2002-04-17
Resolution : 2.55 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
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

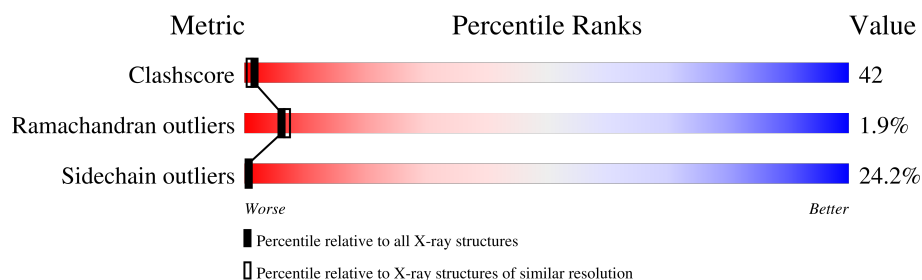
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

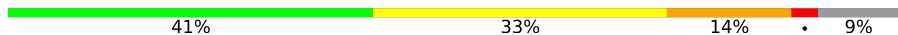
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)

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	363	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2631 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.

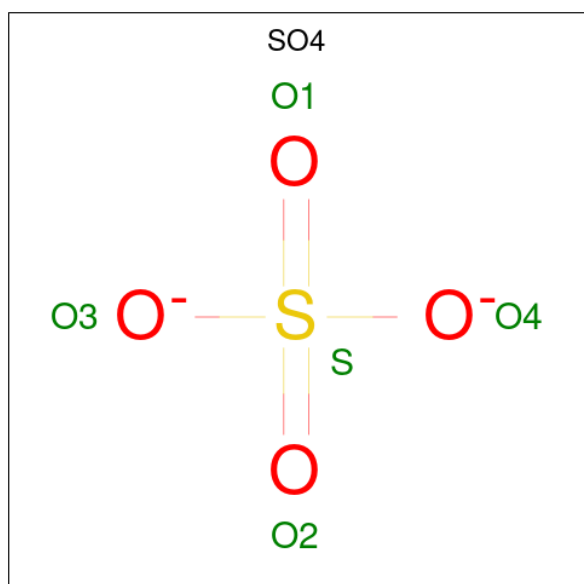
- Molecule 1 is a protein called adenosine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	330	2433	1546	415	457	15	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	THR	VAL	conflict	UNP Q9TVW2
A	150	ILE	LEU	conflict	UNP Q9TVW2
A	153	ASN	ASP	conflict	UNP Q9TVW2
A	242	VAL	THR	conflict	UNP Q9TVW2
A	246	VAL	THR	conflict	UNP Q9TVW2
A	327	GLY	ALA	conflict	UNP Q9TVW2

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

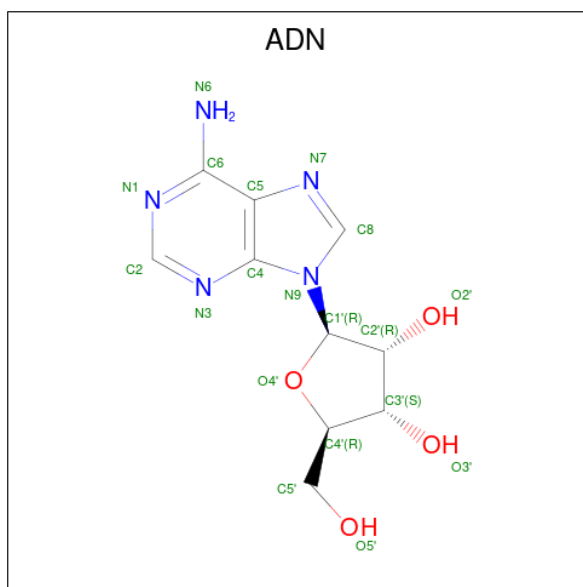


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is ADENOSINE (CCD ID: ADN) (formula: C₁₀H₁₃N₅O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			19	10	5	4		
4	A	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 5 is water.

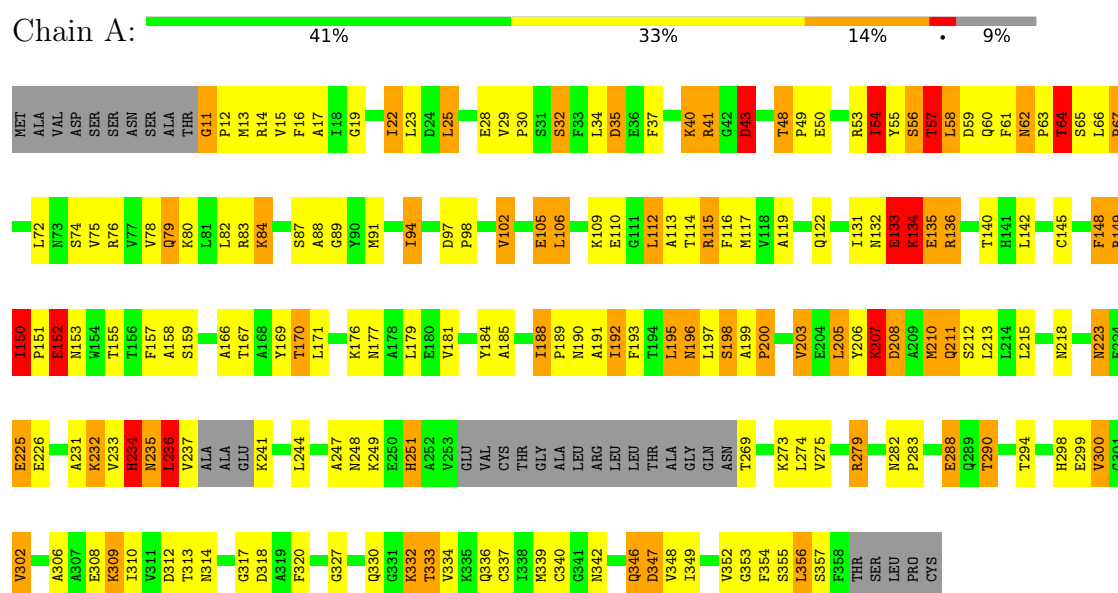
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	154	Total	O	0	0
			154	154		

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: adenosine kinase



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	168.20Å 47.01Å 44.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.55	Depositor
% Data completeness (in resolution range)	99.0 (10.00-2.55)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.150 , 0.200	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2631	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: CL, SO4, ADN

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	3.79	16/2478 (0.6%)	2.16	48/3366 (1.4%)

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

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

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	THR	CB-OG1	131.67	3.54	1.43
1	A	269	THR	C-O	90.12	3.03	1.23
1	A	269	THR	CB-CG2	65.55	3.68	1.52
1	A	152	GLU	CD-OE2	51.75	2.23	1.25
1	A	152	GLU	CG-CD	-18.02	1.07	1.52
1	A	152	GLU	CD-OE1	13.93	1.51	1.25
1	A	151	PRO	C-N	11.21	1.49	1.33
1	A	152	GLU	C-N	9.14	1.45	1.33
1	A	150	ILE	CA-CB	8.53	1.65	1.54
1	A	153	ASN	N-CA	7.73	1.55	1.46
1	A	151	PRO	C-O	7.16	1.32	1.23
1	A	170	THR	CA-CB	7.04	1.65	1.53
1	A	54	ILE	CA-CB	6.78	1.62	1.54
1	A	290	THR	CA-CB	-6.26	1.43	1.53
1	A	248	ASN	CA-CB	-6.00	1.43	1.53
1	A	234	HIS	N-CA	-5.61	1.39	1.46

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	THR	CA-CB-OG1	-50.40	34.01	109.60
1	A	269	THR	CA-CB-CG2	-46.13	32.08	110.50
1	A	269	THR	CA-C-O	-40.29	52.31	120.80
1	A	269	THR	OG1-CB-CG2	-35.14	39.01	109.30
1	A	300	VAL	CB-CA-C	10.56	124.00	110.91
1	A	152	GLU	N-CA-CB	10.24	127.79	110.49
1	A	151	PRO	O-C-N	8.75	133.85	123.01
1	A	203	VAL	CB-CA-C	-7.83	101.79	112.04
1	A	150	ILE	CB-CA-C	7.39	124.81	111.36
1	A	234	HIS	CB-CA-C	7.33	125.00	110.42
1	A	188	ILE	CB-CA-C	-7.31	102.89	110.71
1	A	153	ASN	N-CA-CB	-7.15	100.04	110.70
1	A	48	THR	N-CA-CB	6.84	117.22	109.49
1	A	57	THR	N-CA-CB	-6.74	99.11	110.49
1	A	134	LYS	N-CA-C	-6.71	104.44	114.64
1	A	356	LEU	CA-C-N	-6.61	113.80	123.05
1	A	356	LEU	C-N-CA	-6.61	113.80	123.05
1	A	112	LEU	CB-CA-C	-6.49	98.55	109.65
1	A	152	GLU	CA-C-N	6.38	133.00	122.73
1	A	152	GLU	C-N-CA	6.38	133.00	122.73
1	A	94	ILE	CB-CA-C	-6.29	103.14	111.70
1	A	241	LYS	CB-CA-C	6.22	121.92	110.10
1	A	203	VAL	N-CA-CB	-6.18	102.74	110.47
1	A	348	VAL	N-CA-C	6.14	116.32	110.42
1	A	114	THR	CB-CA-C	-6.12	96.62	110.07
1	A	140	THR	N-CA-C	6.04	119.39	109.72
1	A	249	LYS	CB-CA-C	5.98	122.94	110.32
1	A	54	ILE	N-CA-CB	5.93	117.89	110.47
1	A	347	ASP	CB-CA-C	5.92	120.17	110.88
1	A	64	THR	CB-CA-C	5.86	120.26	109.71
1	A	167	THR	CB-CA-C	-5.66	100.46	109.80
1	A	148	PHE	N-CA-CB	5.59	118.15	109.48
1	A	153	ASN	N-CA-C	5.46	118.95	112.72
1	A	346	GLN	CB-CA-C	5.41	119.38	110.88
1	A	67	PRO	CB-CA-C	-5.35	104.77	111.56
1	A	181	VAL	CB-CA-C	-5.35	104.92	112.14
1	A	43	ASP	N-CA-CB	-5.34	102.63	110.26
1	A	135	GLU	CB-CA-C	-5.30	99.72	109.46
1	A	340	CYS	N-CA-CB	5.29	117.89	110.12
1	A	273	LYS	CB-CA-C	5.27	119.10	111.82
1	A	62	ASN	CB-CA-C	5.26	114.94	111.20
1	A	22	ILE	N-CA-CB	-5.22	103.67	112.44
1	A	11	GLY	C-N-CD	-5.21	103.66	125.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	GLU	CB-CA-C	-5.16	102.23	110.79
1	A	54	ILE	CG1-CB-CG2	-5.12	95.33	110.70
1	A	251	HIS	CB-CA-C	-5.12	100.52	110.46
1	A	195	LEU	N-CA-CB	-5.12	102.01	111.53
1	A	356	LEU	N-CA-C	5.02	120.25	113.72

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	241	LYS	CA

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	2433	0	2400	204	0
2	A	5	0	0	0	0
3	A	1	0	0	0	0
4	A	38	0	26	1	0
5	A	154	0	0	27	0
All	All	2631	0	2426	204	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 42.

All (204) 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:196:ASN:HD22	1:A:198:SER:H	1.01	0.97
1:A:41:ARG:HH11	1:A:132:ASN:ND2	1.62	0.97
1:A:333:THR:HG23	1:A:336:GLN:NE2	1.83	0.93
1:A:207:LYS:HD3	1:A:207:LYS:H	1.34	0.90
1:A:196:ASN:ND2	1:A:198:SER:H	1.68	0.90
1:A:79:GLN:HE22	1:A:87:SER:H	1.15	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ARG:HH11	1:A:136:ARG:HG3	1.39	0.88
1:A:232:LYS:HA	1:A:237:VAL:HG12	1.54	0.87
1:A:333:THR:H	1:A:336:GLN:HE21	1.20	0.86
1:A:171:LEU:HB2	1:A:206:TYR:CD1	2.13	0.83
1:A:193:PHE:H	1:A:218:ASN:ND2	1.76	0.82
1:A:192:ILE:HG13	1:A:218:ASN:HB2	1.62	0.82
1:A:152:GLU:CD	1:A:152:GLU:OE2	2.23	0.81
1:A:223:ASN:ND2	1:A:226:GLU:H	1.78	0.81
1:A:41:ARG:NH1	1:A:132:ASN:ND2	2.29	0.81
1:A:333:THR:HG23	1:A:336:GLN:HE21	1.45	0.80
1:A:231:ALA:HA	1:A:236:LEU:CD1	2.11	0.80
1:A:306:ALA:H	1:A:309:LYS:HZ3	1.29	0.79
1:A:66:LEU:HA	5:A:1039:HOH:O	1.88	0.74
1:A:66:LEU:HB2	1:A:67:PRO:HD2	1.69	0.74
1:A:233:VAL:HG12	1:A:234:HIS:CD2	2.23	0.73
1:A:225:GLU:HG2	1:A:226:GLU:N	2.00	0.73
1:A:79:GLN:HE22	1:A:87:SER:N	1.85	0.73
1:A:179:LEU:HD23	1:A:213:LEU:HD13	1.71	0.73
1:A:41:ARG:HH11	1:A:132:ASN:HD22	1.36	0.73
1:A:60:GLN:HB3	5:A:1011:HOH:O	1.87	0.72
1:A:236:LEU:CB	1:A:247:ALA:HB1	2.19	0.72
1:A:150:ILE:HG22	1:A:177:ASN:OD1	1.89	0.72
1:A:274:LEU:HD13	1:A:288:GLU:HB2	1.70	0.72
1:A:91:MET:HE3	1:A:157:PHE:CD2	2.25	0.71
1:A:136:ARG:HD3	1:A:314:ASN:HA	1.71	0.71
1:A:148:PHE:O	1:A:149:ARG:HD3	1.90	0.71
1:A:188:ILE:CG2	1:A:191:ALA:HB2	2.21	0.71
1:A:231:ALA:HA	1:A:236:LEU:HD12	1.71	0.71
1:A:309:LYS:HB2	1:A:309:LYS:NZ	2.01	0.70
1:A:342:ASN:O	1:A:346:GLN:HG3	1.92	0.69
1:A:88:ALA:HB1	5:A:1120:HOH:O	1.90	0.69
1:A:215:LEU:HD23	1:A:251:HIS:O	1.92	0.69
1:A:333:THR:H	1:A:336:GLN:NE2	1.91	0.69
1:A:306:ALA:HB3	1:A:309:LYS:CE	2.23	0.69
1:A:188:ILE:HG23	1:A:189:PRO:HD2	1.76	0.68
1:A:11:GLY:O	1:A:14:ARG:HD2	1.94	0.68
1:A:306:ALA:N	1:A:309:LYS:NZ	2.42	0.67
1:A:64:THR:HG21	5:A:1010:HOH:O	1.93	0.67
1:A:171:LEU:HA	5:A:1132:HOH:O	1.93	0.67
1:A:235:ASN:O	1:A:237:VAL:N	2.28	0.67
1:A:206:TYR:HA	5:A:1065:HOH:O	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ASN:N	1:A:235:ASN:OD1	2.29	0.66
1:A:179:LEU:CD2	1:A:213:LEU:HD13	2.26	0.66
1:A:207:LYS:NZ	5:A:1016:HOH:O	2.30	0.65
1:A:306:ALA:N	1:A:309:LYS:HZ3	1.93	0.65
1:A:223:ASN:HD21	1:A:226:GLU:HG3	1.61	0.65
1:A:40:LYS:HZ2	1:A:41:ARG:H	1.43	0.65
1:A:306:ALA:HB3	1:A:309:LYS:NZ	2.11	0.65
1:A:190:ASN:HB3	5:A:1092:HOH:O	1.97	0.64
1:A:355:SER:HB3	5:A:1123:HOH:O	1.96	0.64
1:A:232:LYS:HA	1:A:237:VAL:CG1	2.27	0.64
1:A:317:GLY:N	5:A:1098:HOH:O	2.30	0.64
1:A:179:LEU:HD23	1:A:213:LEU:CD1	2.28	0.62
1:A:306:ALA:H	1:A:309:LYS:NZ	1.97	0.62
1:A:309:LYS:HB2	1:A:309:LYS:HZ1	1.63	0.62
1:A:193:PHE:H	1:A:218:ASN:HD22	1.46	0.62
1:A:233:VAL:HG12	1:A:234:HIS:HD2	1.63	0.62
1:A:76:ARG:HD2	1:A:110:GLU:OE2	1.98	0.62
1:A:35:ASP:N	1:A:35:ASP:OD1	2.30	0.61
1:A:223:ASN:C	1:A:223:ASN:HD22	2.09	0.61
1:A:236:LEU:HB3	1:A:247:ALA:HB1	1.83	0.61
1:A:203:VAL:HA	1:A:210:MET:HE1	1.82	0.60
1:A:115:ARG:NH1	5:A:1047:HOH:O	2.34	0.60
1:A:312:ASP:OD1	1:A:353:GLY:N	2.29	0.60
1:A:206:TYR:O	1:A:210:MET:HB2	2.02	0.60
1:A:236:LEU:HB2	1:A:247:ALA:HB1	1.85	0.59
1:A:41:ARG:NH1	1:A:132:ASN:HD21	2.00	0.59
1:A:200:PRO:O	1:A:203:VAL:HB	2.03	0.59
1:A:37:PHE:CE2	1:A:53:ARG:HB3	2.38	0.59
1:A:279:ARG:HB2	1:A:282:ASN:HB2	1.84	0.59
1:A:188:ILE:HB	1:A:191:ALA:CB	2.32	0.59
1:A:223:ASN:HD21	1:A:226:GLU:H	1.50	0.59
1:A:188:ILE:HG21	1:A:191:ALA:HB2	1.85	0.58
1:A:327:GLY:O	1:A:330:GLN:HB2	2.03	0.58
1:A:136:ARG:HH11	1:A:136:ARG:CG	2.13	0.57
1:A:312:ASP:CG	1:A:353:GLY:H	2.11	0.57
1:A:37:PHE:HE2	1:A:53:ARG:HB3	1.69	0.57
1:A:48:THR:HB	1:A:49:PRO:CD	2.35	0.57
1:A:66:LEU:HB2	1:A:67:PRO:CD	2.34	0.57
1:A:22:ILE:HD11	1:A:142:LEU:HD23	1.87	0.56
1:A:184:TYR:O	1:A:188:ILE:HD13	2.06	0.56
1:A:136:ARG:HG3	1:A:136:ARG:O	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ARG:HH11	1:A:279:ARG:HG3	1.71	0.56
1:A:41:ARG:HG2	1:A:135:GLU:HG3	1.88	0.56
1:A:205:LEU:O	1:A:207:LYS:HD3	2.06	0.56
1:A:197:LEU:O	1:A:199:ALA:N	2.38	0.54
1:A:236:LEU:HD23	1:A:236:LEU:N	2.21	0.54
1:A:15:VAL:HG21	1:A:78:VAL:HG11	1.88	0.54
1:A:298:HIS:HD2	5:A:1042:HOH:O	1.90	0.54
1:A:89:GLY:HA2	1:A:113:ALA:O	2.06	0.54
1:A:196:ASN:HD22	1:A:198:SER:N	1.86	0.54
1:A:211:GLN:HG3	1:A:234:HIS:HE1	1.72	0.54
1:A:74:SER:O	1:A:78:VAL:HG23	2.07	0.54
1:A:166:ALA:O	1:A:195:LEU:HD12	2.08	0.53
1:A:313:THR:HA	1:A:349:ILE:HG22	1.89	0.53
1:A:231:ALA:HA	1:A:236:LEU:HD11	1.90	0.53
1:A:53:ARG:NH2	5:A:1029:HOH:O	2.41	0.52
1:A:192:ILE:HG13	1:A:218:ASN:CB	2.36	0.52
1:A:37:PHE:CD1	1:A:54:ILE:HG22	2.44	0.52
1:A:60:GLN:HE21	1:A:61:PHE:HE1	1.55	0.52
1:A:188:ILE:HB	1:A:191:ALA:HB3	1.91	0.52
1:A:54:ILE:HD13	1:A:55:TYR:N	2.24	0.52
1:A:207:LYS:HD3	1:A:207:LYS:N	2.14	0.52
1:A:333:THR:O	1:A:337:CYS:N	2.41	0.51
1:A:208:ASP:OD1	1:A:208:ASP:N	2.43	0.51
1:A:119:ALA:HB1	1:A:122:GLN:OE1	2.10	0.51
1:A:40:LYS:O	1:A:43:ASP:HB2	2.11	0.51
1:A:41:ARG:HH11	1:A:132:ASN:HD21	1.49	0.51
1:A:279:ARG:HG3	1:A:279:ARG:NH1	2.26	0.51
1:A:171:LEU:HD23	5:A:1132:HOH:O	2.11	0.51
1:A:225:GLU:HB3	5:A:1063:HOH:O	2.11	0.51
1:A:66:LEU:HD23	1:A:66:LEU:N	2.26	0.51
1:A:59:ASP:C	1:A:61:PHE:H	2.18	0.50
1:A:53:ARG:O	1:A:57:THR:OG1	2.29	0.50
1:A:274:LEU:HD12	1:A:275:VAL:H	1.77	0.50
1:A:40:LYS:NZ	1:A:41:ARG:H	2.10	0.49
1:A:290:THR:OG1	1:A:294:THR:HB	2.12	0.49
1:A:223:ASN:HD22	1:A:226:GLU:H	1.58	0.49
1:A:142:LEU:HD22	1:A:145:CYS:CB	2.43	0.49
1:A:354:PHE:N	5:A:1059:HOH:O	2.45	0.49
1:A:11:GLY:N	5:A:1094:HOH:O	2.45	0.49
1:A:134:LYS:HE3	1:A:310:ILE:O	2.12	0.49
1:A:17:ALA:HB3	1:A:75:VAL:HG11	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:VAL:O	1:A:106:LEU:HD23	2.13	0.48
1:A:79:GLN:NE2	1:A:87:SER:N	2.58	0.48
1:A:132:ASN:O	1:A:133:GLU:HB2	2.13	0.48
1:A:72:LEU:HG	5:A:1148:HOH:O	2.13	0.48
1:A:98:PRO:HD2	5:A:1037:HOH:O	2.12	0.48
1:A:309:LYS:HG2	5:A:1135:HOH:O	2.14	0.48
1:A:12:PRO:O	1:A:87:SER:HA	2.14	0.47
1:A:196:ASN:HD22	1:A:197:LEU:N	2.12	0.47
1:A:28:GLU:HA	1:A:131:ILE:O	2.13	0.47
1:A:19:GLY:HA2	1:A:170:THR:CG2	2.44	0.47
1:A:50:GLU:HB2	5:A:1055:HOH:O	2.14	0.47
1:A:312:ASP:OD1	1:A:352:VAL:HA	2.14	0.47
1:A:330:GLN:NE2	1:A:330:GLN:HA	2.30	0.47
1:A:211:GLN:HG3	1:A:234:HIS:CE1	2.50	0.47
1:A:231:ALA:HB1	1:A:237:VAL:O	2.13	0.46
1:A:37:PHE:CG	1:A:54:ILE:CG2	2.98	0.46
1:A:274:LEU:HD13	1:A:288:GLU:CB	2.44	0.46
1:A:40:LYS:HD2	1:A:40:LYS:HA	1.17	0.46
1:A:54:ILE:HD11	1:A:55:TYR:CE1	2.51	0.46
1:A:60:GLN:HG3	1:A:61:PHE:CD1	2.51	0.46
1:A:54:ILE:CD1	1:A:55:TYR:N	2.78	0.46
1:A:84:LYS:HZ3	1:A:84:LYS:HG2	1.46	0.46
1:A:198:SER:HA	5:A:1106:HOH:O	2.16	0.46
1:A:302:VAL:HG12	5:A:1152:HOH:O	2.15	0.46
1:A:40:LYS:CE	1:A:41:ARG:N	2.79	0.46
1:A:152:GLU:CD	5:A:1119:HOH:O	2.58	0.46
1:A:195:LEU:HD12	1:A:196:ASN:H	1.81	0.45
1:A:12:PRO:HG2	1:A:13:MET:H	1.82	0.45
1:A:279:ARG:NH1	1:A:283:PRO:O	2.46	0.45
1:A:57:THR:O	1:A:60:GLN:HG2	2.17	0.45
1:A:166:ALA:O	1:A:195:LEU:HA	2.17	0.45
1:A:207:LYS:H	1:A:207:LYS:CD	2.04	0.45
1:A:60:GLN:CG	1:A:61:PHE:CE1	3.00	0.45
1:A:79:GLN:NE2	1:A:87:SER:H	1.97	0.44
1:A:306:ALA:CB	1:A:309:LYS:NZ	2.80	0.44
1:A:169:TYR:CD1	1:A:198:SER:HB3	2.52	0.44
1:A:37:PHE:CG	1:A:54:ILE:HG22	2.53	0.44
1:A:54:ILE:CD1	1:A:55:TYR:H	2.30	0.44
1:A:155:THR:HG23	5:A:1127:HOH:O	2.17	0.44
1:A:25:LEU:HD12	1:A:25:LEU:HA	1.74	0.44
1:A:142:LEU:HD22	1:A:145:CYS:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:PRO:HB2	1:A:32:SER:OG	2.18	0.43
1:A:179:LEU:HD23	1:A:179:LEU:HA	1.37	0.43
1:A:223:ASN:HD21	1:A:225:GLU:HG2	1.83	0.43
1:A:206:TYR:N	1:A:206:TYR:CD2	2.80	0.43
1:A:60:GLN:CG	1:A:61:PHE:CD1	3.02	0.43
1:A:136:ARG:HG3	1:A:136:ARG:NH1	2.15	0.43
1:A:72:LEU:HB3	5:A:1148:HOH:O	2.20	0.42
1:A:185:ALA:O	1:A:191:ALA:HB3	2.19	0.42
1:A:60:GLN:HG3	1:A:61:PHE:CE1	2.55	0.42
1:A:188:ILE:CB	1:A:191:ALA:HB2	2.49	0.42
1:A:332:LYS:HA	1:A:332:LYS:HD2	1.79	0.42
1:A:75:VAL:HB	5:A:1120:HOH:O	2.19	0.42
1:A:97:ASP:HB2	1:A:98:PRO:HD2	2.02	0.42
1:A:207:LYS:HB2	1:A:208:ASP:H	1.75	0.42
1:A:235:ASN:HB2	1:A:236:LEU:H	1.60	0.42
1:A:318:ASP:OD2	4:A:699:ADN:O5'	2.36	0.42
1:A:356:LEU:HD23	1:A:356:LEU:HA	1.74	0.42
1:A:79:GLN:HE21	1:A:88:ALA:H	1.67	0.42
1:A:231:ALA:O	1:A:235:ASN:O	2.38	0.41
1:A:283:PRO:HA	1:A:300:VAL:O	2.20	0.41
1:A:54:ILE:CD1	1:A:55:TYR:CD1	3.04	0.41
1:A:223:ASN:ND2	1:A:225:GLU:CD	2.79	0.41
1:A:72:LEU:O	1:A:76:ARG:HG3	2.21	0.41
1:A:312:ASP:OD2	1:A:353:GLY:HA2	2.20	0.41
1:A:317:GLY:O	1:A:320:PHE:HB3	2.21	0.41
1:A:196:ASN:HD22	1:A:196:ASN:C	2.28	0.41
1:A:244:LEU:O	1:A:247:ALA:HB3	2.21	0.41
1:A:94:ILE:HG23	1:A:116:PHE:CD2	2.56	0.41
1:A:306:ALA:HB3	1:A:309:LYS:HE3	2.02	0.40
1:A:59:ASP:C	1:A:61:PHE:N	2.79	0.40
1:A:62:ASN:N	1:A:63:PRO:CD	2.83	0.40
1:A:16:PHE:CD1	1:A:158:ALA:HB2	2.56	0.40
1:A:56:SER:C	1:A:58:LEU:N	2.79	0.40
1:A:188:ILE:HD12	1:A:188:ILE:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	323/363 (89%)	293 (91%)	24 (7%)	6 (2%)	6 7

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	LEU
1	A	133	GLU
1	A	198	SER
1	A	207	LYS
1	A	234	HIS
1	A	57	THR

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	252/287 (88%)	191 (76%)	61 (24%)	1 1

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	25	LEU
1	A	29	VAL
1	A	32	SER
1	A	34	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	35	ASP
1	A	40	LYS
1	A	41	ARG
1	A	43	ASP
1	A	54	ILE
1	A	56	SER
1	A	57	THR
1	A	58	LEU
1	A	64	THR
1	A	65	SER
1	A	79	GLN
1	A	80	LYS
1	A	82	LEU
1	A	83	ARG
1	A	84	LYS
1	A	102	VAL
1	A	105	GLU
1	A	106	LEU
1	A	109	LYS
1	A	112	LEU
1	A	115	ARG
1	A	117	MET
1	A	133	GLU
1	A	134	LYS
1	A	136	ARG
1	A	149	ARG
1	A	150	ILE
1	A	152	GLU
1	A	159	SER
1	A	176	LYS
1	A	192	ILE
1	A	196	ASN
1	A	200	PRO
1	A	205	LEU
1	A	207	LYS
1	A	208	ASP
1	A	210	MET
1	A	211	GLN
1	A	212	SER
1	A	223	ASN
1	A	225	GLU
1	A	232	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	235	ASN
1	A	236	LEU
1	A	279	ARG
1	A	288	GLU
1	A	299	GLU
1	A	302	VAL
1	A	308	GLU
1	A	309	LYS
1	A	332	LYS
1	A	333	THR
1	A	334	VAL
1	A	339	MET
1	A	347	ASP
1	A	357	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	79	GLN
1	A	101	GLN
1	A	132	ASN
1	A	141	HIS
1	A	186	HIS
1	A	190	ASN
1	A	196	ASN
1	A	218	ASN
1	A	223	ASN
1	A	229	HIS
1	A	234	HIS
1	A	298	HIS
1	A	314	ASN
1	A	330	GLN
1	A	336	GLN
1	A	342	ASN
1	A	346	GLN
1	A	350	GLN
1	A	351	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, 1 is monoatomic - leaving 3 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	$\# Z > 2$
4	ADN	A	799	-	21,21,21	0.27	0	31,31,31	0.64	0
4	ADN	A	699	-	21,21,21	0.60	0	31,31,31	0.67	0
2	SO4	A	999	-	4,4,4	0.69	0	6,6,6	0.17	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADN	A	799	-	-	0/6/22/22	0/3/3/3
4	ADN	A	699	-	-	0/6/22/22	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	699	ADN	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	269:THR	C	270:GLY	N	3.61

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.