



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:07 AM UTC

PDB ID : 3ADK / pdb_00003adk
Title : REFINED STRUCTURE OF PORCINE CYTOSOLIC ADENYLATE KINASE AT 2.1 ANGSTROMS RESOLUTION
Authors : Schulz, G.E.
Deposited on : 1987-11-19
Resolution : 2.10 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

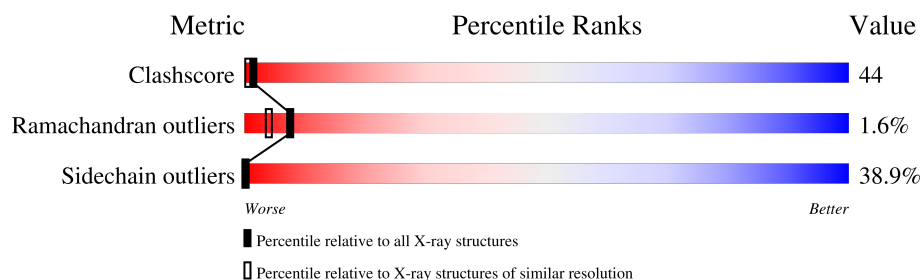
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	195	24% 34% 31% 11%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1529 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 ADENYLATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1519	955	260	296	8			

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



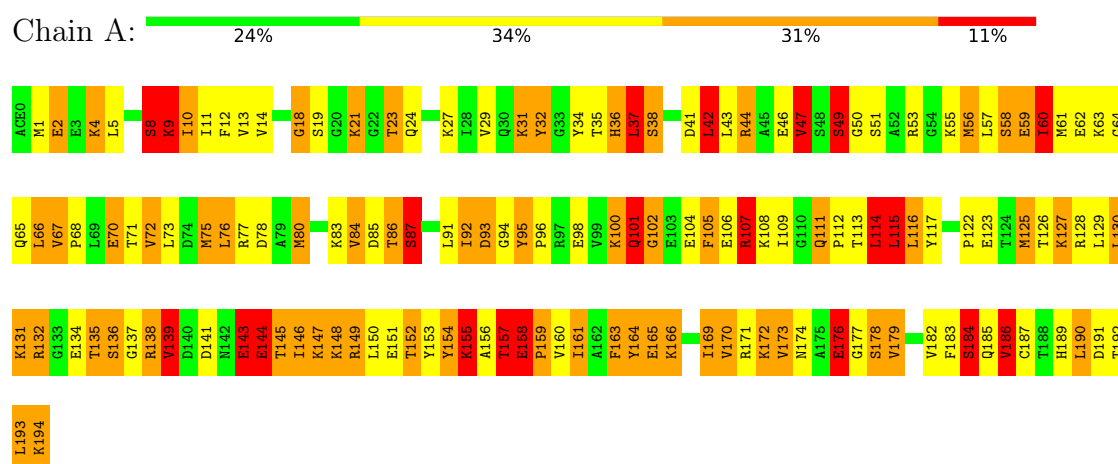
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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: ADENYLATE KINASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	48.50Å 48.50Å 141.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1529	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: SO4, ACE

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	1.95	37/1536 (2.4%)	2.30	74/2057 (3.6%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	VAL	CA-C	-8.87	1.42	1.52
1	A	177	GLY	C-N	-8.69	1.22	1.33
1	A	37	LEU	C-N	6.92	1.42	1.33
1	A	4	LYS	N-CA	-6.61	1.38	1.46
1	A	95	TYR	CA-C	-6.49	1.44	1.52
1	A	157	THR	CA-C	-6.18	1.45	1.52
1	A	59	GLU	N-CA	-6.06	1.38	1.46
1	A	86	THR	CA-C	6.03	1.60	1.52
1	A	10	ILE	C-O	-6.00	1.17	1.24
1	A	170	VAL	CA-C	-5.84	1.45	1.52
1	A	146	ILE	CA-C	-5.75	1.46	1.52
1	A	18	GLY	CA-C	5.65	1.59	1.51
1	A	135	THR	N-CA	-5.64	1.39	1.46
1	A	42	LEU	C-O	-5.62	1.17	1.24
1	A	8	SER	C-N	-5.58	1.25	1.33
1	A	9	LYS	N-CA	-5.57	1.39	1.46
1	A	58	SER	C-N	-5.53	1.25	1.33
1	A	144	GLU	CA-C	-5.47	1.45	1.52
1	A	31	LYS	CA-C	-5.46	1.47	1.53
1	A	150	LEU	CA-C	-5.38	1.46	1.52
1	A	164	TYR	CA-C	5.38	1.59	1.52
1	A	21	LYS	N-CA	-5.33	1.39	1.46
1	A	72	VAL	CA-C	-5.32	1.46	1.52
1	A	150	LEU	C-O	-5.32	1.18	1.24
1	A	135	THR	C-O	-5.28	1.17	1.24
1	A	76	LEU	CA-C	5.25	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	LEU	CA-C	-5.20	1.46	1.52
1	A	78	ASP	CG-OD2	5.20	1.35	1.25
1	A	151	GLU	CD-OE2	5.16	1.35	1.25
1	A	41	ASP	CG-OD2	5.15	1.35	1.25
1	A	157	THR	N-CA	-5.12	1.40	1.46
1	A	75	MET	N-CA	-5.11	1.40	1.46
1	A	38	SER	CA-C	-5.11	1.46	1.52
1	A	158	GLU	CD-OE2	5.10	1.35	1.25
1	A	122	PRO	CA-C	5.10	1.59	1.52
1	A	152	THR	C-O	-5.02	1.17	1.24
1	A	49	SER	CA-C	-5.00	1.46	1.52

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	ASP	CA-CB-CG	11.84	124.44	112.60
1	A	191	ASP	CA-CB-CG	-11.01	101.59	112.60
1	A	139	VAL	N-CA-CB	-9.51	95.53	111.23
1	A	93	ASP	CA-CB-CG	-8.77	103.83	112.60
1	A	151	GLU	CB-CG-CD	-8.12	98.79	112.60
1	A	13	VAL	CB-CA-C	-7.87	101.80	111.32
1	A	146	ILE	N-CA-CB	7.58	118.58	110.62
1	A	113	THR	N-CA-CB	-7.45	99.10	110.20
1	A	164	TYR	N-CA-C	7.11	119.11	111.36
1	A	36	HIS	O-C-N	-7.07	114.64	123.05
1	A	184	SER	CA-C-N	7.07	129.75	120.28
1	A	184	SER	C-N-CA	7.07	129.75	120.28
1	A	93	ASP	CB-CA-C	-7.06	99.67	110.26
1	A	63	LYS	N-CA-C	-6.99	104.76	113.28
1	A	50	GLY	N-CA-C	-6.82	105.46	115.63
1	A	93	ASP	N-CA-C	6.76	119.53	109.59
1	A	37	LEU	CA-C-O	-6.57	113.27	120.30
1	A	47	VAL	N-CA-CB	6.57	117.80	110.51
1	A	60	ILE	CA-C-N	6.46	128.83	120.44
1	A	60	ILE	C-N-CA	6.46	128.83	120.44
1	A	159	PRO	N-CA-CB	6.43	108.37	101.88
1	A	87	SER	N-CA-C	6.41	118.99	110.53
1	A	143	GLU	N-CA-C	-6.40	103.55	112.25
1	A	32	TYR	N-CA-C	6.23	120.14	112.54
1	A	155	LYS	N-CA-C	6.21	117.72	111.07
1	A	107	ARG	O-C-N	6.20	129.30	122.11
1	A	80	MET	N-CA-CB	6.11	119.72	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	PHE	N-CA-C	-6.07	104.75	111.36
1	A	107	ARG	CA-C-N	6.04	131.71	121.14
1	A	107	ARG	C-N-CA	6.04	131.71	121.14
1	A	53	ARG	CA-C-N	5.96	130.99	120.74
1	A	53	ARG	C-N-CA	5.96	130.99	120.74
1	A	146	ILE	O-C-N	5.95	128.38	121.96
1	A	151	GLU	CB-CA-C	-5.92	100.95	110.79
1	A	59	GLU	CB-CG-CD	-5.92	102.53	112.60
1	A	172	LYS	N-CA-CB	5.92	119.93	110.16
1	A	38	SER	CB-CA-C	-5.92	98.73	109.38
1	A	186	VAL	CA-CB-CG2	5.91	120.45	110.40
1	A	112	PRO	N-CA-CB	5.87	108.23	103.36
1	A	2	GLU	N-CA-CB	5.86	118.50	110.01
1	A	102	GLY	N-CA-C	-5.85	107.41	114.66
1	A	136	SER	N-CA-C	5.76	120.43	113.17
1	A	84	VAL	N-CA-C	5.75	118.28	111.09
1	A	13	VAL	CA-C-O	-5.74	113.23	120.69
1	A	38	SER	N-CA-CB	5.73	119.92	110.69
1	A	134	GLU	CB-CA-C	-5.73	101.88	110.88
1	A	130	LEU	CA-C-N	5.70	128.38	120.29
1	A	130	LEU	C-N-CA	5.70	128.38	120.29
1	A	21	LYS	CB-CA-C	5.66	121.92	110.38
1	A	75	MET	CA-C-N	5.55	127.99	120.44
1	A	75	MET	C-N-CA	5.55	127.99	120.44
1	A	92	ILE	CA-C-N	5.54	129.22	121.24
1	A	92	ILE	C-N-CA	5.54	129.22	121.24
1	A	176	GLU	N-CA-CB	5.51	119.20	110.55
1	A	12	PHE	CA-CB-CG	5.50	119.30	113.80
1	A	112	PRO	CB-CA-C	-5.49	104.69	111.11
1	A	132	ARG	CD-NE-CZ	5.46	132.05	124.40
1	A	101	GLN	N-CA-CB	-5.45	101.93	110.44
1	A	172	LYS	N-CA-C	5.28	118.22	109.46
1	A	194	LYS	N-CA-CB	5.25	119.42	110.50
1	A	60	ILE	CA-CB-CG2	5.24	119.41	110.50
1	A	114	LEU	CA-C-N	-5.24	115.41	122.86
1	A	114	LEU	C-N-CA	-5.24	115.41	122.86
1	A	100	LYS	CA-C-O	5.15	125.75	119.05
1	A	154	TYR	N-CA-C	-5.13	105.77	111.36
1	A	31	LYS	CA-C-N	5.12	129.28	120.72
1	A	31	LYS	C-N-CA	5.12	129.28	120.72
1	A	135	THR	O-C-N	-5.07	116.42	122.20
1	A	144	GLU	O-C-N	5.06	129.27	122.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ILE	CA-CB-CG2	5.05	119.08	110.50
1	A	75	MET	O-C-N	5.04	127.46	122.12
1	A	60	ILE	CA-CB-CG1	5.04	118.97	110.40
1	A	10	ILE	N-CA-C	5.04	115.10	107.80
1	A	86	THR	N-CA-CB	-5.01	103.92	110.59

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	1519	0	1565	136	0
2	A	10	0	0	0	0
All	All	1529	0	1565	136	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 44.

All (136) 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:19:SER:HB3	1:A:125:MET:HE2	1.44	0.98
1:A:44:ARG:HB2	1:A:44:ARG:NH1	1.79	0.97
1:A:9:LYS:HZ1	1:A:194:LYS:HE3	1.33	0.93
1:A:1:MET:HE3	1:A:1:MET:HA	1.50	0.92
1:A:9:LYS:NZ	1:A:194:LYS:HG2	1.86	0.89
1:A:58:SER:O	1:A:62:GLU:HG3	1.73	0.88
1:A:107:ARG:HB3	1:A:107:ARG:NH1	1.89	0.88
1:A:144:GLU:O	1:A:148:LYS:HB2	1.77	0.85
1:A:152:THR:HA	1:A:155:LYS:HD3	1.62	0.82
1:A:44:ARG:HB2	1:A:44:ARG:HH11	1.43	0.81
1:A:27:LYS:HE3	1:A:179:VAL:CG2	2.12	0.79
1:A:9:LYS:HZ3	1:A:194:LYS:HG2	1.46	0.79
1:A:27:LYS:HE3	1:A:179:VAL:HG23	1.65	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:TYR:O	1:A:158:GLU:HG3	1.84	0.78
1:A:114:LEU:HD22	1:A:115:LEU:N	1.98	0.77
1:A:114:LEU:HD22	1:A:115:LEU:H	1.47	0.76
1:A:71:THR:O	1:A:75:MET:HG3	1.86	0.75
1:A:31:LYS:HD2	1:A:32:TYR:CE1	2.22	0.75
1:A:161:ILE:O	1:A:165:GLU:HG2	1.87	0.74
1:A:170:VAL:O	1:A:171:ARG:HD2	1.87	0.74
1:A:107:ARG:HB3	1:A:107:ARG:HH11	1.47	0.74
1:A:11:ILE:HD11	1:A:34:TYR:CE1	2.23	0.73
1:A:96:PRO:HB3	1:A:101:GLN:HG2	1.71	0.73
1:A:43:LEU:HD22	1:A:61:MET:CE	2.20	0.71
1:A:83:LYS:O	1:A:87:SER:HB2	1.91	0.71
1:A:129:LEU:HB3	1:A:146:ILE:CD1	2.20	0.70
1:A:46:GLU:O	1:A:49:SER:HB2	1.91	0.70
1:A:9:LYS:HZ1	1:A:194:LYS:CE	2.04	0.69
1:A:60:ILE:HD11	1:A:68:PRO:HD3	1.74	0.69
1:A:44:ARG:HH11	1:A:44:ARG:CB	2.06	0.69
1:A:67:VAL:HG13	1:A:68:PRO:HD2	1.73	0.69
1:A:9:LYS:NZ	1:A:194:LYS:HE3	2.08	0.68
1:A:1:MET:HE1	1:A:4:LYS:HD2	1.76	0.68
1:A:43:LEU:O	1:A:47:VAL:HG23	1.93	0.68
1:A:71:THR:HG22	1:A:75:MET:HE2	1.76	0.67
1:A:171:ARG:HB3	1:A:189:HIS:CD2	2.30	0.67
1:A:171:ARG:HG2	1:A:189:HIS:HD2	1.63	0.64
1:A:153:TYR:CD1	1:A:157:THR:HB	2.32	0.64
1:A:36:HIS:HA	1:A:91:LEU:HB3	1.80	0.64
1:A:184:SER:O	1:A:187:CYS:HB2	1.98	0.64
1:A:174:ASN:OD1	1:A:176:GLU:HG2	1.97	0.63
1:A:1:MET:CE	1:A:4:LYS:HB3	2.29	0.62
1:A:19:SER:HB3	1:A:125:MET:CE	2.26	0.62
1:A:116:LEU:HD11	1:A:173:VAL:HG13	1.83	0.61
1:A:183:PHE:HA	1:A:186:VAL:HG13	1.84	0.60
1:A:190:LEU:O	1:A:193:LEU:HB2	2.01	0.59
1:A:96:PRO:HG3	1:A:102:GLY:HA2	1.84	0.59
1:A:143:GLU:O	1:A:147:LYS:HB2	2.02	0.58
1:A:35:THR:HG22	1:A:37:LEU:HD13	1.86	0.58
1:A:43:LEU:HD22	1:A:61:MET:HE2	1.86	0.58
1:A:60:ILE:HD11	1:A:67:VAL:HA	1.86	0.58
1:A:72:VAL:HA	1:A:75:MET:HE3	1.85	0.57
1:A:44:ARG:NH1	1:A:44:ARG:CB	2.61	0.57
1:A:98:GLU:O	1:A:101:GLN:HB3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:VAL:O	1:A:164:TYR:HD1	1.89	0.56
1:A:73:LEU:HD11	1:A:104:GLU:HB3	1.87	0.56
1:A:31:LYS:HB3	1:A:32:TYR:CD1	2.42	0.55
1:A:1:MET:HE3	1:A:4:LYS:HB3	1.88	0.54
1:A:5:LEU:O	1:A:8:SER:HB2	2.08	0.54
1:A:60:ILE:O	1:A:65:GLN:HB2	2.08	0.53
1:A:145:THR:O	1:A:149:ARG:N	2.38	0.53
1:A:9:LYS:HD2	1:A:34:TYR:OH	2.09	0.52
1:A:60:ILE:CD1	1:A:68:PRO:HD3	2.40	0.52
1:A:145:THR:O	1:A:149:ARG:HB2	2.09	0.51
1:A:186:VAL:HG23	1:A:190:LEU:HD22	1.91	0.51
1:A:70:GLU:HG3	1:A:71:THR:N	2.25	0.51
1:A:129:LEU:HB3	1:A:146:ILE:HD13	1.90	0.51
1:A:1:MET:CE	1:A:4:LYS:HD2	2.41	0.50
1:A:170:VAL:C	1:A:171:ARG:HD2	2.36	0.50
1:A:178:SER:O	1:A:182:VAL:HG23	2.11	0.50
1:A:67:VAL:HG13	1:A:68:PRO:CD	2.42	0.50
1:A:123:GLU:O	1:A:127:LYS:HD2	2.12	0.49
1:A:152:THR:O	1:A:155:LYS:HG2	2.12	0.49
1:A:157:THR:O	1:A:159:PRO:N	2.45	0.49
1:A:1:MET:HA	1:A:1:MET:CE	2.35	0.49
1:A:9:LYS:HD2	1:A:193:LEU:HD23	1.93	0.48
1:A:43:LEU:HD23	1:A:57:LEU:HD13	1.94	0.48
1:A:182:VAL:O	1:A:186:VAL:HG13	2.13	0.48
1:A:35:THR:HG22	1:A:37:LEU:CD1	2.43	0.48
1:A:129:LEU:CB	1:A:146:ILE:CD1	2.89	0.48
1:A:1:MET:HE1	1:A:84:VAL:HG11	1.96	0.47
1:A:44:ARG:HB2	1:A:44:ARG:CZ	2.44	0.47
1:A:106:GLU:HG2	1:A:111:GLN:HA	1.96	0.47
1:A:94:GLY:O	1:A:95:TYR:HB2	2.14	0.47
1:A:9:LYS:CE	1:A:194:LYS:HE3	2.45	0.47
1:A:80:MET:HE1	1:A:109:ILE:HG21	1.95	0.47
1:A:43:LEU:HD22	1:A:61:MET:HE1	1.93	0.47
1:A:11:ILE:CD1	1:A:34:TYR:CE1	2.97	0.46
1:A:67:VAL:HA	1:A:68:PRO:HD3	1.68	0.46
1:A:73:LEU:HD21	1:A:95:TYR:OH	2.16	0.46
1:A:77:ARG:HG3	1:A:109:ILE:HG12	1.96	0.45
1:A:96:PRO:HG3	1:A:102:GLY:CA	2.46	0.45
1:A:56:MET:O	1:A:60:ILE:HG23	2.17	0.45
1:A:61:MET:O	1:A:64:GLY:HA2	2.17	0.45
1:A:166:LYS:HA	1:A:166:LYS:HD2	1.40	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLY:O	1:A:128:ARG:NE	2.28	0.44
1:A:101:GLN:HE21	1:A:101:GLN:HB2	1.38	0.44
1:A:105:PHE:C	1:A:105:PHE:CD2	2.95	0.44
1:A:169:ILE:HD13	1:A:169:ILE:HG21	1.65	0.44
1:A:11:ILE:HD13	1:A:11:ILE:HG21	1.84	0.43
1:A:92:ILE:HG22	1:A:95:TYR:HB3	1.99	0.43
1:A:171:ARG:CG	1:A:189:HIS:CD2	3.02	0.43
1:A:116:LEU:HD11	1:A:173:VAL:CG1	2.47	0.43
1:A:153:TYR:CE1	1:A:157:THR:HB	2.53	0.43
1:A:23:THR:O	1:A:27:LYS:HG3	2.19	0.43
1:A:31:LYS:HD2	1:A:32:TYR:CZ	2.54	0.43
1:A:131:LYS:HG2	1:A:132:ARG:N	2.32	0.43
1:A:11:ILE:HD12	1:A:91:LEU:HD12	2.01	0.43
1:A:157:THR:C	1:A:159:PRO:HD2	2.43	0.43
1:A:24:GLN:NE2	1:A:24:GLN:HA	2.33	0.42
1:A:95:TYR:CG	1:A:96:PRO:HA	2.54	0.42
1:A:130:LEU:HA	1:A:130:LEU:HD23	1.76	0.42
1:A:161:ILE:HG23	1:A:161:ILE:HD13	1.46	0.42
1:A:158:GLU:N	1:A:159:PRO:CD	2.83	0.42
1:A:186:VAL:HG23	1:A:190:LEU:CD2	2.49	0.42
1:A:171:ARG:HH21	1:A:171:ARG:HD3	1.60	0.42
1:A:163:PHE:C	1:A:163:PHE:CD1	2.98	0.42
1:A:129:LEU:HD23	1:A:129:LEU:HA	1.92	0.41
1:A:9:LYS:HZ1	1:A:194:LYS:HG2	1.76	0.41
1:A:95:TYR:HA	1:A:96:PRO:C	2.45	0.41
1:A:139:VAL:H	1:A:139:VAL:HG13	0.92	0.41
1:A:100:LYS:HE2	1:A:100:LYS:HB3	1.97	0.41
1:A:171:ARG:CB	1:A:189:HIS:CD2	3.01	0.41
1:A:174:ASN:H	1:A:185:GLN:HE22	1.68	0.41
1:A:11:ILE:HD11	1:A:34:TYR:HE1	1.80	0.41
1:A:96:PRO:CG	1:A:102:GLY:CA	2.99	0.41
1:A:114:LEU:CD2	1:A:115:LEU:H	2.24	0.41
1:A:137:GLY:O	1:A:139:VAL:HG12	2.20	0.41
1:A:171:ARG:CG	1:A:189:HIS:HD2	2.28	0.41
1:A:156:ALA:C	1:A:159:PRO:HD2	2.46	0.41
1:A:161:ILE:HG21	1:A:161:ILE:HD12	1.50	0.41
1:A:42:LEU:HA	1:A:42:LEU:HD12	1.63	0.40
1:A:66:LEU:C	1:A:66:LEU:HD23	2.46	0.40
1:A:182:VAL:O	1:A:182:VAL:HG12	2.20	0.40
1:A:9:LYS:CE	1:A:194:LYS:HG2	2.49	0.40
1:A:117:TYR:C	1:A:117:TYR:CD2	2.99	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	193/195 (99%)	176 (91%)	14 (7%)	3 (2%)	7 4

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	ARG
1	A	158	GLU
1	A	139	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	167/167 (100%)	102 (61%)	65 (39%)	0 0

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	8	SER
1	A	9	LYS
1	A	10	ILE
1	A	14	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	21	LYS
1	A	23	THR
1	A	29	VAL
1	A	37	LEU
1	A	38	SER
1	A	42	LEU
1	A	44	ARG
1	A	47	VAL
1	A	49	SER
1	A	51	SER
1	A	55	LYS
1	A	56	MET
1	A	59	GLU
1	A	60	ILE
1	A	66	LEU
1	A	67	VAL
1	A	70	GLU
1	A	76	LEU
1	A	86	THR
1	A	87	SER
1	A	93	ASP
1	A	101	GLN
1	A	105	PHE
1	A	107	ARG
1	A	108	LYS
1	A	111	GLN
1	A	114	LEU
1	A	115	LEU
1	A	116	LEU
1	A	125	MET
1	A	126	THR
1	A	127	LYS
1	A	131	LYS
1	A	135	THR
1	A	136	SER
1	A	138	ARG
1	A	139	VAL
1	A	141	ASP
1	A	143	GLU
1	A	144	GLU
1	A	145	THR
1	A	147	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	148	LYS
1	A	149	ARG
1	A	155	LYS
1	A	157	THR
1	A	158	GLU
1	A	161	ILE
1	A	165	GLU
1	A	166	LYS
1	A	172	LYS
1	A	173	VAL
1	A	176	GLU
1	A	178	SER
1	A	179	VAL
1	A	184	SER
1	A	186	VAL
1	A	190	LEU
1	A	192	THR
1	A	193	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	101	GLN
1	A	142	ASN
1	A	185	GLN
1	A	189	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	195	-	4,4,4	0.30	0	6,6,6	0.40	0
2	SO4	A	196	-	4,4,4	0.71	0	6,6,6	0.35	0

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.

No monomer is involved in short contacts.

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

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.