



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:35 PM UTC

PDB ID : 1ADE / pdb_00001ade
Title : STRUCTURE OF ADENYLOSUCCINATE SYNTHETASE PH 7 AT 25 DEGREES CELSIUS
Authors : Silva, M.M.; Poland, B.W.; Hoffman, C.M.; Fromm, H.J.; Honzatko, R.B.
Deposited on : 1995-09-14
Resolution : 2.00 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
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

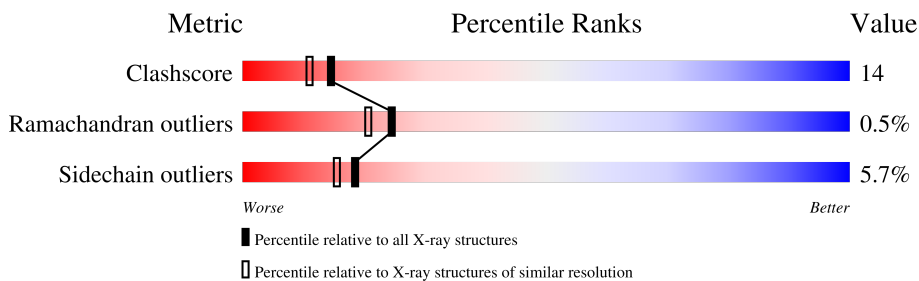
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	431	 68% 28% .
1	B	431	 67% 29% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9988 atoms, of which 2677 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 ADENYLOSUCCINATE SYNTHETASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	431	Total	C	H	N	O	S	0	6	0
			4150	2128	771	592	646	13			
1	B	431	Total	C	H	N	O	S	0	4	0
			4116	2114	758	585	646	13			

- Molecule 2 is water.

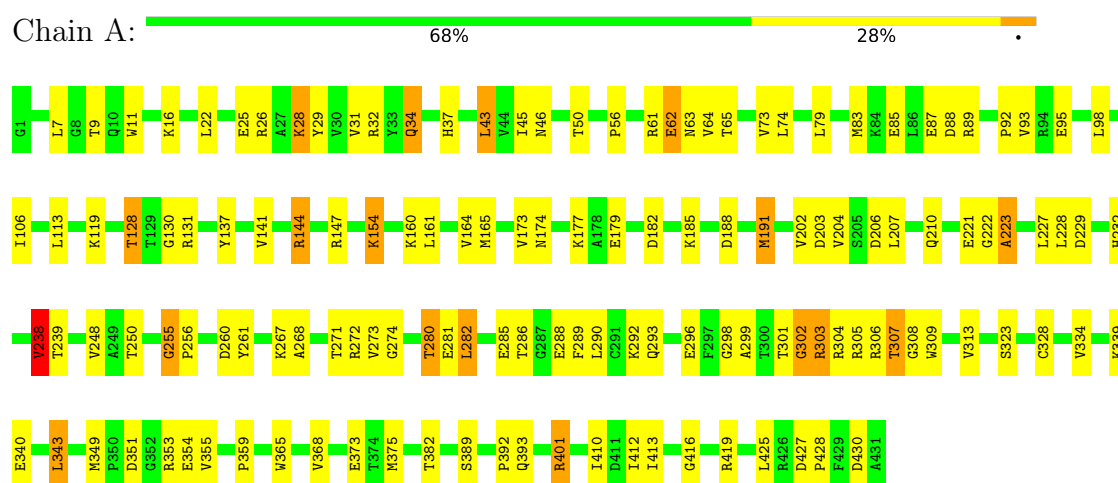
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	314	Total	H	O	0	0
			942	628	314		
2	B	260	Total	H	O	0	0
			780	520	260		

3 Residue-property plots

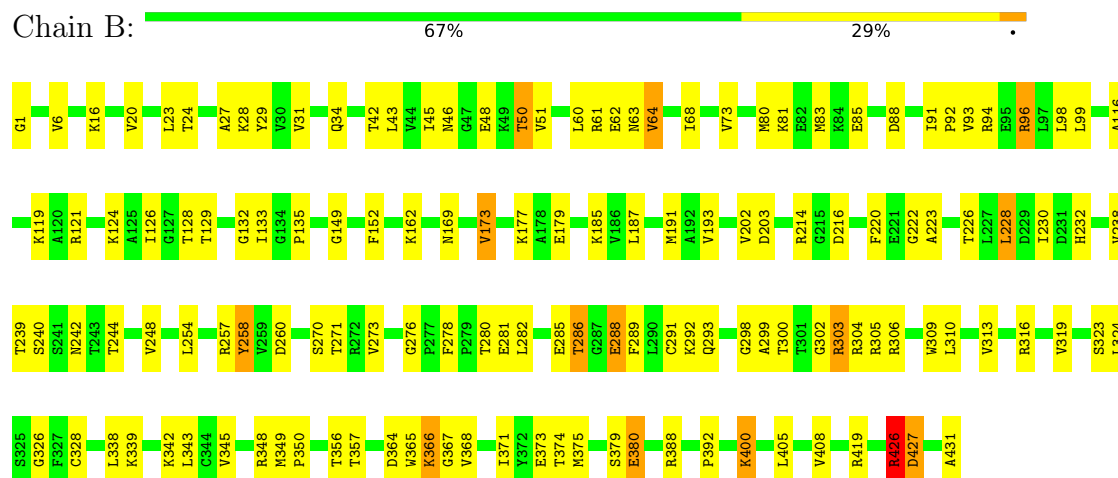
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: ADENYLOSUCCINATE SYNTHETASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.26Å 72.18Å 82.90Å 90.00° 108.17° 90.00°	Depositor
Resolution (Å)	5.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9988	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.68	0/3437	1.15	27/4649 (0.6%)
1	B	0.66	0/3416	1.11	24/4624 (0.5%)
All	All	0.67	0/6853	1.13	51/9273 (0.5%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	GLY	N-CA-C	15.13	132.78	110.38
1	A	301	THR	N-CA-C	8.44	121.69	110.88
1	A	223	ALA	N-CA-C	7.89	119.96	111.36
1	A	299	ALA	N-CA-C	7.35	121.90	112.34
1	B	31	VAL	N-CA-C	7.30	118.33	108.11
1	B	232	HIS	N-CA-C	6.99	121.97	113.38
1	B	276	GLY	CA-C-N	6.96	127.34	119.83
1	B	276	GLY	C-N-CA	6.96	127.34	119.83
1	A	255	GLY	CA-C-N	6.94	127.23	119.32
1	A	255	GLY	C-N-CA	6.94	127.23	119.32
1	A	238	VAL	N-CA-CB	-6.79	104.51	112.32
1	B	223	ALA	N-CA-C	6.64	122.19	113.30
1	A	174	ASN	N-CA-C	6.55	119.40	111.40
1	B	278	PHE	CA-C-N	6.45	126.14	119.56
1	B	278	PHE	C-N-CA	6.45	126.14	119.56
1	A	74	LEU	N-CA-C	6.41	118.73	108.41
1	B	313	VAL	N-CA-C	-6.40	104.62	110.82
1	A	232	HIS	N-CA-C	6.39	120.78	112.92
1	A	62	GLU	N-CA-C	6.29	118.70	111.02
1	A	154	LYS	N-CA-C	6.22	118.06	111.28
1	B	173	VAL	N-CA-C	6.22	116.85	110.82
1	B	373	GLU	N-CA-C	-6.15	98.39	108.41
1	B	64	VAL	N-CA-C	6.07	118.09	108.87
1	A	328	CYS	N-CA-C	-6.06	98.53	108.41
1	B	328	CYS	N-CA-C	-6.04	97.45	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	ARG	N-CA-C	-6.00	104.61	113.61
1	A	31	VAL	N-CA-C	5.98	116.73	108.12
1	B	242	ASN	N-CA-C	-5.96	100.78	110.20
1	B	93	VAL	N-CA-C	5.94	116.59	110.36
1	B	248	VAL	N-CA-C	5.89	116.08	110.42
1	A	260	ASP	N-CA-C	5.88	118.58	111.40
1	A	301	THR	CA-C-N	-5.88	113.28	120.92
1	A	301	THR	C-N-CA	-5.88	113.28	120.92
1	B	303	ARG	N-CA-C	5.68	117.48	108.79
1	B	62	GLU	N-CA-C	5.53	118.24	111.82
1	B	357	THR	N-CA-C	-5.49	101.22	109.95
1	B	258	TYR	N-CA-C	5.47	118.96	112.72
1	A	313	VAL	N-CA-C	-5.47	105.39	110.53
1	A	268	ALA	N-CA-C	5.38	118.94	112.38
1	B	427	ASP	CA-C-N	5.30	125.37	119.32
1	B	427	ASP	C-N-CA	5.30	125.37	119.32
1	A	373	GLU	N-CA-C	-5.29	99.15	108.20
1	A	9	THR	N-CA-C	5.26	119.84	113.38
1	A	204	VAL	N-CA-C	5.26	115.98	110.62
1	A	355	VAL	N-CA-C	5.24	116.92	108.85
1	A	93	VAL	N-CA-C	5.15	115.36	110.42
1	A	416	GLY	CA-C-N	5.15	124.65	119.19
1	A	416	GLY	C-N-CA	5.15	124.65	119.19
1	B	426	ARG	N-CA-C	5.13	121.22	114.75
1	B	260	ASP	N-CA-C	5.04	119.46	112.45
1	B	228	LEU	N-CA-C	-5.01	106.58	113.30

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	3379	771	3398	98	4
1	B	3358	758	3365	94	2
2	A	314	628	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	260	520	0	15	0
All	All	7311	2677	6763	189	4

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 (189) 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:296:GLU:O	1:A:305:ARG:HG2	1.77	0.84
1:B:273:VAL:HG11	1:B:300:THR:OG1	1.79	0.82
1:A:272:ARG:HH11	1:A:272:ARG:HG2	1.46	0.81
1:A:303:ARG:HD3	1:A:303:ARG:H	1.50	0.77
1:A:28:LYS:NZ	1:A:28:LYS:HB2	2.02	0.75
1:B:350:PRO:HG3	1:B:367:GLY:HA3	1.69	0.74
1:B:375:MET:SD	2:B:625:HOH:O	2.45	0.74
1:A:288:GLU:O	1:A:292[A]:LYS:HG2	1.88	0.74
1:B:46:ASN:HD21	1:B:91:ILE:HD11	1.51	0.73
1:A:290:LEU:HB2	1:A:307:THR:HG21	1.70	0.73
1:B:42:THR:HG22	1:B:51:VAL:HG22	1.70	0.72
1:B:285:GLU:O	1:B:288:GLU:HG3	1.89	0.72
1:A:191:MET:HE3	1:A:191:MET:HA	1.70	0.71
1:A:343:LEU:HD21	1:A:375:MET:HE3	1.73	0.70
1:A:228:LEU:O	1:A:239:THR:HG22	1.91	0.69
1:A:25:GLU:HG2	1:A:61[B]:ARG:NH1	2.09	0.68
1:A:375:MET:HE1	1:A:401:ARG:HG3	1.77	0.67
1:A:274:GLY:H	1:A:304:ARG:HB3	1.60	0.66
1:B:73:VAL:HG21	1:B:133:ILE:HG23	1.76	0.66
1:A:83:MET:O	1:A:87:GLU:HG2	1.96	0.66
1:B:126:ILE:O	1:B:128:THR:HG23	1.95	0.65
1:B:280:THR:HG21	1:B:309:TRP:O	1.96	0.65
1:B:28:LYS:HD2	1:B:29:TYR:CE2	2.31	0.65
1:A:280:THR:HG21	1:A:309:TRP:O	1.96	0.65
1:B:298:GLY:HA2	1:B:303:ARG:O	1.98	0.64
1:A:98:LEU:HD13	1:A:202:VAL:HG11	1.81	0.63
1:B:349:MET:HE1	1:B:368:VAL:HG12	1.80	0.63
1:B:230:ILE:HD12	1:B:240:SER:HA	1.82	0.61
1:A:273:VAL:HG11	1:A:302:GLY:HA3	1.81	0.61
1:A:289:PHE:HB2	2:A:693:HOH:O	2.00	0.60
1:B:400:LYS:O	1:B:400:LYS:HE3	2.02	0.59
1:B:342:LYS:HG2	1:B:374:THR:HG22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:VAL:CG2	1:B:300:THR:HG21	2.32	0.58
1:A:16[B]:LYS:HE2	1:A:222:GLY:O	2.04	0.58
1:A:419[A]:ARG:HD2	1:A:419[A]:ARG:H	1.68	0.58
1:B:426:ARG:HH11	1:B:426:ARG:HB2	1.69	0.57
1:A:191:MET:HA	1:A:191:MET:CE	2.35	0.57
1:B:349:MET:CE	1:B:368:VAL:HG12	2.35	0.57
1:A:173:VAL:O	1:A:177[A]:LYS:HA	2.05	0.57
1:A:206:ASP:O	1:A:210:GLN:HG2	2.05	0.57
1:A:293:GLN:HB2	1:A:334:VAL:HG13	1.87	0.56
1:B:116:ALA:HA	1:B:119:LYS:HD3	1.88	0.56
1:B:191:MET:HE2	1:B:191:MET:HA	1.86	0.56
1:B:345:VAL:HG12	1:B:405:LEU:HD13	1.87	0.56
1:B:365:TRP:O	1:B:368:VAL:HG22	2.05	0.56
1:B:94:ARG:HB3	2:B:565:HOH:O	2.05	0.56
1:B:426:ARG:O	1:B:426:ARG:HG3	2.05	0.55
1:A:227:LEU:HD11	2:A:565:HOH:O	2.06	0.55
1:B:173:VAL:O	1:B:177[A]:LYS:HA	2.06	0.55
1:A:43:LEU:HD13	1:A:45:ILE:HG13	1.89	0.55
1:A:128:THR:HG23	1:A:130:GLY:H	1.72	0.54
1:B:83:MET:SD	2:B:549:HOH:O	2.59	0.54
1:B:46:ASN:ND2	1:B:91:ILE:HD11	2.19	0.54
1:B:426:ARG:HB2	1:B:426:ARG:NH1	2.22	0.54
1:B:316:ARG:NH1	1:B:356:THR:O	2.39	0.54
1:A:323:SER:O	1:B:257:ARG:NH1	2.41	0.53
1:A:128:THR:HG23	1:A:130:GLY:N	2.23	0.53
1:A:161:LEU:O	1:A:165:MET:HG3	2.08	0.53
1:A:248:VAL:HB	2:A:663:HOH:O	2.07	0.52
1:A:282:LEU:HD22	1:A:308:GLY:HA2	1.91	0.52
1:A:61[A]:ARG:NE	1:A:64:VAL:HG23	2.25	0.52
1:A:281:GLU:OE2	1:A:306:ARG:HD2	2.10	0.51
1:B:80:MET:HG3	1:B:193:VAL:HG11	1.91	0.51
1:A:16[B]:LYS:NZ	1:A:221:GLU:OE2	2.43	0.51
1:A:61[A]:ARG:HE	1:A:64:VAL:HG23	1.76	0.51
1:B:173:VAL:O	1:B:177[B]:LYS:HA	2.09	0.51
1:B:119:LYS:NZ	2:B:641:HOH:O	2.42	0.51
1:A:296:GLU:C	1:A:298:GLY:H	2.18	0.51
1:A:92:PRO:HB2	1:A:95:GLU:HG2	1.91	0.51
1:A:349:MET:HE1	1:A:368:VAL:CG1	2.40	0.51
1:B:350:PRO:HG2	1:B:364:ASP:OD2	2.10	0.51
1:A:272:ARG:HH11	1:A:272:ARG:CG	2.16	0.50
1:B:1:GLY:H1	1:B:431:ALA:C	2.16	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:GLY:O	1:B:303:ARG:HG3	2.11	0.50
1:A:303:ARG:O	1:A:304:ARG:HB2	2.11	0.50
1:B:364:ASP:OD1	1:B:366:LYS:HG3	2.11	0.50
1:A:37:HIS:O	1:A:131:ARG:NH1	2.44	0.50
1:B:220:PHE:CZ	1:B:254:LEU:HD22	2.48	0.49
1:A:280:THR:HG23	1:A:280:THR:O	2.12	0.49
1:B:20:VAL:O	1:B:24:THR:HG23	2.11	0.49
1:B:350:PRO:HG3	1:B:367:GLY:CA	2.42	0.49
1:A:85:GLU:O	1:A:89:ARG:HD3	2.13	0.49
1:B:63:ASN:HA	2:B:511:HOH:O	2.12	0.49
1:B:88:ASP:HA	2:B:562:HOH:O	2.13	0.49
1:A:289:PHE:CE1	1:A:293:GLN:NE2	2.81	0.49
1:A:255:GLY:HA3	1:B:323:SER:HB3	1.95	0.49
1:B:282:LEU:HD13	1:B:286:THR:HB	1.94	0.49
1:A:61[A]:ARG:HH22	1:A:63:ASN:HB2	1.78	0.48
1:B:380:GLU:HG3	1:B:392:PRO:HB3	1.95	0.48
1:B:187:LEU:O	1:B:191:MET:HG2	2.13	0.48
1:A:274:GLY:N	1:A:304:ARG:HB3	2.26	0.48
1:B:419[A]:ARG:NH1	2:B:663:HOH:O	2.46	0.48
1:B:214:ARG:HD2	1:B:216:ASP:OD2	2.13	0.48
1:B:45:ILE:N	1:B:48:GLU:O	2.46	0.47
1:B:68:ILE:HB	1:B:99:LEU:HD23	1.97	0.47
1:B:326:GLY:HA2	1:B:408:VAL:CG1	2.44	0.47
1:B:273:VAL:HG22	1:B:305:ARG:HG3	1.97	0.47
1:A:28:LYS:HB2	1:A:28:LYS:HZ2	1.77	0.47
1:A:177[A]:LYS:HG2	2:A:487:HOH:O	2.15	0.47
1:A:349:MET:HE1	1:A:368:VAL:HG12	1.95	0.47
1:B:203:ASP:HB3	2:B:559:HOH:O	2.14	0.47
1:B:273:VAL:HG22	1:B:300:THR:HG21	1.97	0.47
1:A:73:VAL:HG13	1:A:137:TYR:CE1	2.50	0.47
1:A:250:THR:HA	2:B:486:HOH:O	2.14	0.47
1:B:281:GLU:OE2	1:B:306:ARG:HD2	2.14	0.47
1:B:273:VAL:HG21	1:B:300:THR:HG21	1.97	0.46
1:A:365:TRP:HA	1:A:368:VAL:HG13	1.97	0.46
1:B:98:LEU:HD13	1:B:202:VAL:HG11	1.97	0.46
1:A:88:ASP:HB2	1:A:89:ARG:HH11	1.79	0.46
1:A:272:ARG:HG2	1:A:272:ARG:NH1	2.23	0.46
1:A:359:PRO:HG2	1:A:365:TRP:CE2	2.50	0.46
1:B:319:VAL:HG22	1:B:324:LEU:HD12	1.98	0.46
1:A:26:ARG:HH12	1:A:430:ASP:CG	2.24	0.46
1:B:126:ILE:O	1:B:126:ILE:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ARG:NH1	1:B:371:ILE:HD11	2.30	0.46
1:A:261:TYR:CE1	1:A:428:PRO:HB3	2.50	0.46
1:B:16:LYS:HE2	1:B:222:GLY:O	2.16	0.45
1:A:62:GLU:CD	1:A:62:GLU:N	2.73	0.45
1:B:380:GLU:H	1:B:380:GLU:CD	2.24	0.45
1:B:61:ARG:HD3	2:B:572:HOH:O	2.15	0.45
1:B:292:LYS:HG3	1:B:293:GLN:N	2.30	0.45
1:B:28:LYS:O	1:B:28:LYS:HD3	2.16	0.45
1:B:285:GLU:H	1:B:285:GLU:CD	2.25	0.45
1:B:149:GLY:O	1:B:152:PHE:HD2	1.99	0.45
1:B:349:MET:HE1	1:B:368:VAL:CG1	2.46	0.44
1:A:410:ILE:O	1:A:425:LEU:HD12	2.17	0.44
1:A:22:LEU:CD1	1:A:419[B]:ARG:HG2	2.48	0.44
1:A:73:VAL:HG23	1:A:106:ILE:HD11	2.00	0.44
1:A:290:LEU:CB	1:A:307:THR:HG21	2.42	0.44
1:B:228:LEU:O	1:B:238:VAL:HB	2.17	0.44
1:B:281:GLU:OE2	1:B:306:ARG:HB3	2.18	0.44
1:A:267:LYS:NZ	1:A:296:GLU:OE2	2.48	0.44
1:A:255:GLY:HA2	1:A:256:PRO:HD3	1.87	0.43
1:B:1:GLY:N	1:B:431:ALA:OXT	2.36	0.43
1:A:343:LEU:N	1:A:343:LEU:HD23	2.34	0.43
1:B:50:THR:HG22	1:B:51:VAL:H	1.82	0.43
1:A:271:THR:HA	1:A:306:ARG:O	2.18	0.43
1:B:132:GLY:C	1:B:135:PRO:HD2	2.44	0.43
1:B:169:ASN:O	1:B:173:VAL:HG22	2.19	0.43
1:B:185:LYS:NZ	2:B:524:HOH:O	2.50	0.43
1:A:29:TYR:CD1	1:A:65:THR:HB	2.54	0.43
1:A:144:ARG:HD3	2:A:649:HOH:O	2.17	0.43
1:A:22:LEU:HD12	1:A:419[B]:ARG:HG2	2.01	0.43
1:A:286:THR:HG21	1:A:309:TRP:CH2	2.53	0.43
1:B:81[A]:LYS:NZ	2:B:531:HOH:O	2.51	0.43
1:B:129:THR:HA	2:B:480:HOH:O	2.18	0.43
1:A:92:PRO:HB2	1:A:95:GLU:CG	2.48	0.42
1:B:280:THR:HG22	2:B:619:HOH:O	2.17	0.42
1:B:6:VAL:HG21	1:B:23:LEU:HD12	2.02	0.42
1:A:11:TRP:CZ2	1:A:227:LEU:HD13	2.54	0.42
1:A:202:VAL:HG22	1:A:203:ASP:N	2.35	0.42
1:A:393:GLN:HB2	2:A:712:HOH:O	2.19	0.42
1:A:43:LEU:HD12	1:A:50:THR:O	2.18	0.42
1:A:349:MET:CE	1:A:368:VAL:HG12	2.50	0.42
1:B:92:PRO:O	1:B:96:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16[A]:LYS:NZ	1:A:223:ALA:O	2.52	0.42
1:B:27:ALA:O	1:B:64:VAL:HG22	2.19	0.42
1:A:412:ILE:HG22	1:A:413:ILE:N	2.35	0.42
1:B:226:THR:HG23	1:B:244:THR:HG22	2.01	0.42
1:B:345:VAL:HG12	1:B:405:LEU:CD1	2.49	0.42
1:A:160:LYS:O	1:A:164:VAL:HG23	2.20	0.42
1:A:323:SER:HB3	1:B:258:TYR:CE2	2.55	0.42
1:B:380:GLU:CG	1:B:392:PRO:HB3	2.49	0.42
1:A:28:LYS:HB2	1:A:28:LYS:HZ3	1.79	0.42
1:A:202:VAL:HG23	2:A:608:HOH:O	2.19	0.42
1:B:45:ILE:HG23	1:B:60:LEU:HD21	2.01	0.41
1:A:32:ARG:HG2	1:A:56:PRO:HG3	2.02	0.41
1:B:121:ARG:HB3	1:B:121:ARG:NH1	2.36	0.41
1:A:286:THR:HG21	1:A:309:TRP:CZ2	2.56	0.41
1:A:289:PHE:O	1:A:293:GLN:HG2	2.19	0.41
1:A:401:ARG:HA	1:A:401:ARG:HD2	1.60	0.41
1:A:61[A]:ARG:HH11	1:A:61[A]:ARG:HG2	1.86	0.41
1:A:154:LYS:HD3	1:A:191:MET:HE2	2.01	0.41
1:A:303:ARG:H	1:A:303:ARG:CD	2.26	0.41
1:B:292:LYS:HD3	2:B:529:HOH:O	2.21	0.41
1:B:310:LEU:HB3	1:B:343:LEU:HD23	2.03	0.41
1:A:229:ASP:O	1:A:238:VAL:CG2	2.69	0.41
1:B:1:GLY:N	1:B:431:ALA:C	2.79	0.41
1:B:85:GLU:O	1:B:88:ASP:HB2	2.21	0.41
1:B:291:CYS:HB2	1:B:304:ARG:HH21	1.86	0.41
1:A:88:ASP:CB	1:A:89:ARG:HH11	2.34	0.40
1:A:382:THR:HG22	1:A:392:PRO:HD2	2.04	0.40
1:A:28:LYS:HG3	1:A:29:TYR:CD2	2.56	0.40
1:A:34:GLN:CD	1:A:34:GLN:C	2.89	0.40
1:B:289:PHE:CD2	1:B:338:LEU:HD21	2.55	0.40
1:A:351:ASP:OD1	1:A:353:ARG:HG2	2.22	0.40
1:B:271:THR:HA	1:B:306:ARG:O	2.22	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LYS:HZ3	1:A:354:GLU:OE2[2_556]	1.38	0.22
1:A:188:ASP:OD2	1:B:292:LYS:HZ3[2_455]	1.39	0.21
1:A:62:GLU:OE1	1:B:388:ARG:HH22[2_555]	1.51	0.09
1:A:182:ASP:OD2	1:A:339:LYS:HZ2[2_556]	1.55	0.05

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	435/431 (101%)	414 (95%)	20 (5%)	1 (0%)	43	42
1	B	433/431 (100%)	411 (95%)	19 (4%)	3 (1%)	18	14
All	All	868/862 (101%)	825 (95%)	39 (4%)	4 (0%)	24	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	124	LYS
1	A	427	ASP
1	B	299	ALA
1	B	427	ASP

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	359/353 (102%)	335 (93%)	24 (7%)	15	11
1	B	357/353 (101%)	341 (96%)	16 (4%)	24	23
All	All	716/706 (101%)	676 (94%)	40 (6%)	18	16

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	28	LYS

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Mol	Chain	Res	Type
1	A	34	GLN
1	A	43	LEU
1	A	46	ASN
1	A	79	LEU
1	A	113	LEU
1	A	128	THR
1	A	141	VAL
1	A	147	ARG
1	A	179	GLU
1	A	185	LYS
1	A	191	MET
1	A	207	LEU
1	A	238	VAL
1	A	280	THR
1	A	282	LEU
1	A	285	GLU
1	A	303	ARG
1	A	307	THR
1	A	340	GLU
1	A	343	LEU
1	A	389	SER
1	A	401	ARG
1	B	34	GLN
1	B	43	LEU
1	B	50	THR
1	B	96	ARG
1	B	162	LYS
1	B	179	GLU
1	B	239	THR
1	B	270	SER
1	B	286	THR
1	B	288	GLU
1	B	339	LYS
1	B	366	LYS
1	B	379	SER
1	B	380	GLU
1	B	400	LYS
1	B	426	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	A	224	GLN
1	B	2	ASN
1	B	46	ASN
1	B	70	ASN
1	B	171	GLN
1	B	293	GLN
1	B	295	ASN

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 ⓘ

There are no ligands in this entry.

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.