



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:21 PM GMT

PDB ID : 1ADI
Title : STRUCTURE OF ADENYLOSUCCINATE SYNTHETASE AT PH 6.5 AND
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 : 2.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

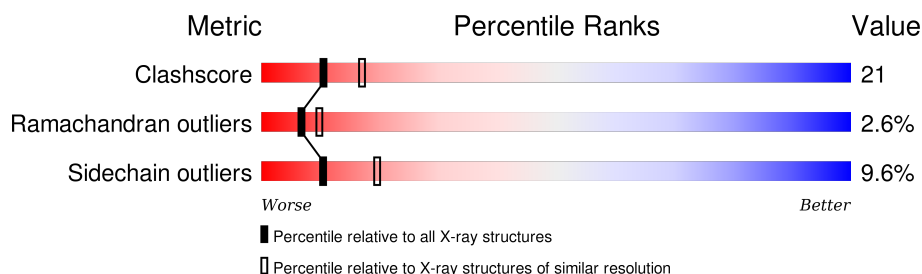
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	431	 59% 35% 6% •
1	B	431	 58% 37% 5% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9584 atoms, of which 2402 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	7	0
			4150	2129	766	590	652	13			
1	B	431	Total	C	H	N	O	S	0	4	0
			4117	2115	758	585	646	13			

- Molecule 2 is water.

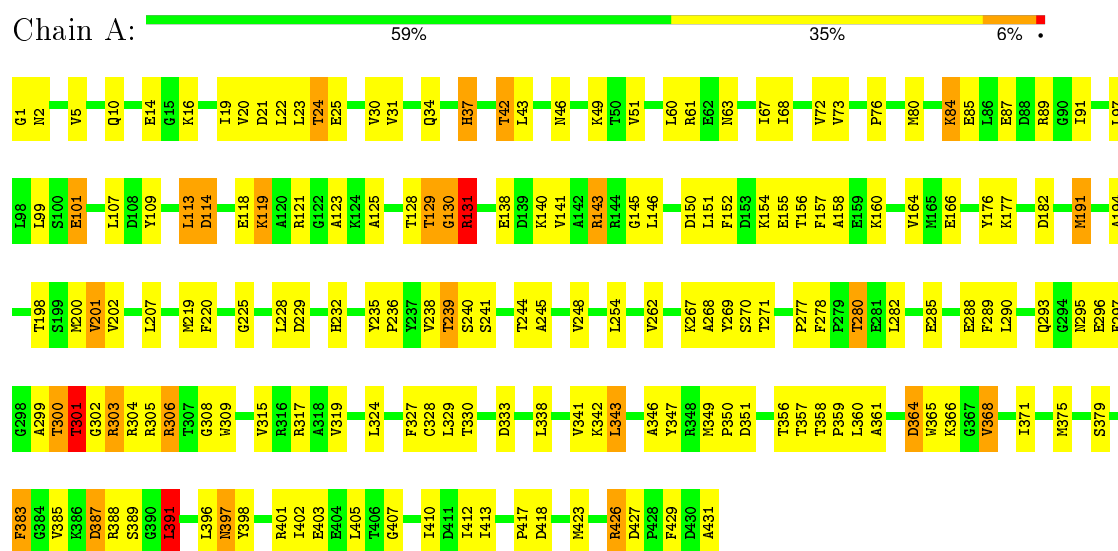
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	223	Total	H	O	0	0
			669	446	223		
2	B	216	Total	H	O	0	0
			648	432	216		

3 Residue-property plots

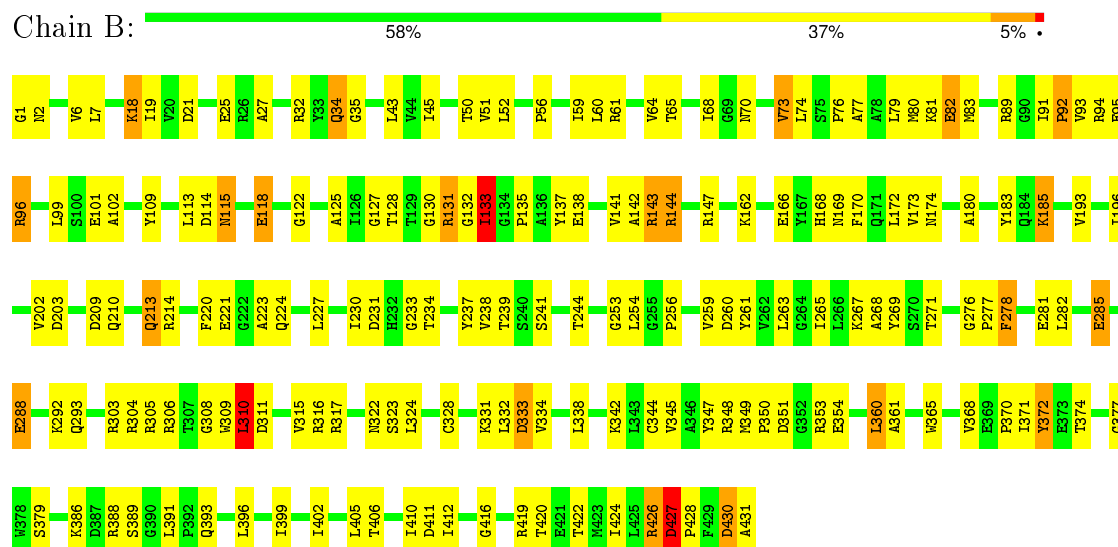
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

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 will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.42Å 93.63Å 119.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.206 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9584	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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	0.69	0/3442	0.89	1/4658 (0.0%)
1	B	0.75	1/3417 (0.0%)	0.96	4/4625 (0.1%)
All	All	0.72	1/6859 (0.0%)	0.93	5/9283 (0.1%)

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	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	221	GLU	CB-CG	-5.33	1.42	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	B	310	LEU	CA-CB-CG	6.41	130.04	115.30
1	A	391	LEU	CA-CB-CG	6.10	129.32	115.30
1	B	427	ASP	CB-CG-OD1	5.65	123.38	118.30
1	B	96	ARG	NE-CZ-NH2	-5.33	117.64	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	235	TYR	Sidechain
1	B	372	TYR	Sidechain

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	3384	766	3387	154	0
1	B	3359	758	3367	145	1
2	A	223	446	0	18	0
2	B	216	432	0	16	0
All	All	7182	2402	6754	289	1

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 21.

All (289) 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:B:43:LEU:HD22	1:B:60:LEU:HD11	1.47	0.96
1:B:342:LYS:HG2	1:B:374:THR:HG22	1.47	0.94
1:A:365:TRP:O	1:A:368:VAL:HG12	1.69	0.93
1:A:296:GLU:HB3	1:A:305:ARG:HD2	1.57	0.84
1:A:140:LYS:HE2	2:A:442:HOH:O	1.77	0.83
1:B:19:ILE:HG12	1:B:328:CYS:SG	2.22	0.80
1:B:360:LEU:HD23	1:B:360:LEU:H	1.49	0.77
1:A:418:ASP:HA	2:A:592:HOH:O	1.84	0.77
1:B:52:LEU:HD22	1:B:82:GLU:HG2	1.67	0.76
1:A:280:THR:HG21	1:A:309:TRP:O	1.87	0.74
1:A:309:TRP:HE1	1:A:342:LYS:HE3	1.53	0.73
1:B:399:ILE:HG23	1:B:410:ILE:HD12	1.70	0.72
1:A:97:LEU:HB3	1:A:200:MET:CE	2.20	0.72
1:A:239:THR:HG23	1:A:241:SER:H	1.53	0.72
1:A:156:THR:O	1:A:160:LYS:HG3	1.91	0.71
1:B:109:TYR:O	1:B:113:LEU:HD13	1.92	0.70
1:B:2:ASN:HB2	2:B:450:HOH:O	1.91	0.70
1:B:285:GLU:HA	1:B:288:GLU:CG	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:PHE:HZ	1:A:201:VAL:HG11	1.56	0.70
1:B:309:TRP:NE1	1:B:342:LYS:HD2	2.08	0.69
1:B:388:ARG:HG2	1:B:388:ARG:HH11	1.59	0.68
1:A:43:LEU:HD23	1:A:60:LEU:HD11	1.75	0.68
1:B:209:ASP:O	1:B:213:GLN:HG2	1.93	0.67
1:A:21:ASP:O	1:A:61:ARG:NH1	2.27	0.67
1:A:85:GLU:O	1:A:89:ARG:HD3	1.95	0.67
1:A:296:GLU:HB3	1:A:305:ARG:CD	2.25	0.67
1:A:359:PRO:HA	2:A:649:HOH:O	1.93	0.66
1:B:45:ILE:HG21	1:B:89:ARG:HD2	1.78	0.66
1:A:119:LYS:HE2	1:A:125:ALA:HB3	1.75	0.66
1:B:285:GLU:HA	1:B:288:GLU:HG2	1.77	0.65
1:B:316:ARG:NH1	1:B:405:LEU:O	2.28	0.65
1:B:292:LYS:HB3	2:B:537:HOH:O	1.96	0.64
1:A:131:ARG:HA	1:A:131:ARG:HE	1.62	0.64
1:B:282:LEU:HG	1:B:308:GLY:HA2	1.81	0.63
1:A:329:LEU:HB2	1:A:410:ILE:HD13	1.80	0.62
1:A:97:LEU:HB3	1:A:200:MET:HE2	1.82	0.62
1:A:87:GLU:HA	1:A:91:ILE:O	2.00	0.62
1:A:288:GLU:HG3	2:A:645:HOH:O	2.00	0.62
1:B:349:MET:CE	1:B:368:VAL:HG22	2.30	0.61
1:B:386:LYS:HE2	1:B:420:THR:O	2.00	0.61
1:B:79:LEU:O	1:B:83:MET:HG3	2.02	0.60
1:A:191:MET:HA	1:A:191:MET:CE	2.32	0.59
1:B:83:MET:HE3	1:B:94:ARG:HG2	1.83	0.59
1:A:19:ILE:HG12	1:A:328:CYS:SG	2.42	0.59
1:B:19:ILE:HD12	1:B:19:ILE:H	1.66	0.59
1:B:277:PRO:HA	2:B:449:HOH:O	2.03	0.59
1:B:115:ASN:O	1:B:118:GLU:HG3	2.02	0.59
1:B:360:LEU:HG	1:B:361:ALA:H	1.68	0.59
1:A:150:ASP:OD1	1:A:160:LYS:HE2	2.03	0.59
1:B:143:ARG:HB3	2:B:586:HOH:O	2.02	0.59
1:B:309:TRP:CE2	1:B:342:LYS:HD2	2.38	0.58
1:B:214:ARG:HD3	2:B:587:HOH:O	2.03	0.58
1:A:76:PRO:O	1:A:80:MET:HG2	2.04	0.57
1:A:43:LEU:O	1:A:49:LYS:HA	2.03	0.57
1:B:411:ASP:O	1:B:412:ILE:HG13	2.04	0.57
1:B:92:PRO:HB2	1:B:95:GLU:HG2	1.87	0.57
1:A:5:VAL:HG21	1:A:248:VAL:HG21	1.85	0.57
1:B:317:ARG:HB2	2:B:645:HOH:O	2.05	0.57
1:A:118:GLU:HB3	1:A:119:LYS:NZ	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:TYR:CD2	1:B:168:HIS:HD2	2.23	0.56
1:B:109:TYR:CD2	1:B:168:HIS:CD2	2.94	0.56
1:A:152:PHE:CZ	1:A:201:VAL:HG11	2.40	0.56
1:B:128:THR:CG2	1:B:131:ARG:HE	2.19	0.55
1:A:299:ALA:O	1:A:300:THR:HG22	2.05	0.55
1:A:42:THR:HG23	1:A:51:VAL:HG22	1.88	0.55
1:B:94:ARG:NH2	1:B:196:ILE:HG23	2.21	0.55
1:A:119:LYS:HE3	1:A:119:LYS:N	2.22	0.55
1:B:311:ASP:HA	1:B:344:CYS:HB3	1.88	0.55
1:A:341:VAL:HG22	1:A:375:MET:O	2.06	0.55
1:A:282:LEU:HG	1:A:308:GLY:HA2	1.90	0.54
1:A:343:LEU:HD12	1:A:405:LEU:CD1	2.37	0.54
1:B:169:ASN:O	1:B:173:VAL:HG13	2.07	0.54
1:B:388:ARG:NH1	1:B:388:ARG:HG2	2.20	0.54
1:B:43:LEU:CD2	1:B:60:LEU:HD11	2.31	0.54
1:A:315:VAL:HA	2:A:568:HOH:O	2.06	0.54
1:B:18:LYS:NZ	1:B:416:GLY:O	2.40	0.54
1:A:278:PHE:HD2	1:A:306:ARG:HG3	1.73	0.54
1:A:305:ARG:N	2:A:566:HOH:O	2.41	0.54
1:A:300:THR:O	1:A:300:THR:HG23	2.08	0.54
1:A:119:LYS:CE	1:A:125:ALA:HB3	2.37	0.53
1:B:94:ARG:CZ	1:B:196:ILE:HG23	2.38	0.53
1:B:193:VAL:HG12	1:B:193:VAL:O	2.08	0.53
1:A:391:LEU:HB3	1:A:396:LEU:CD1	2.38	0.53
1:A:146:LEU:HD22	1:A:157:PHE:CE1	2.44	0.53
1:A:25:GLU:HG3	1:A:61:ARG:CZ	2.39	0.53
1:B:348:ARG:CZ	1:B:371:ILE:HD11	2.38	0.53
1:A:84:LYS:HE2	2:A:562:HOH:O	2.09	0.53
1:A:398:TYR:O	1:A:402:ILE:HG13	2.09	0.53
1:A:19:ILE:CD1	1:A:328:CYS:SG	2.97	0.52
1:B:210:GLN:NE2	2:B:523:HOH:O	2.41	0.52
1:A:285:GLU:OE1	1:A:285:GLU:HA	2.08	0.52
1:A:301:THR:OG1	1:A:302:GLY:N	2.41	0.52
1:A:277:PRO:HB3	1:A:365:TRP:HB3	1.91	0.52
1:B:64:VAL:CG1	1:B:65:THR:N	2.73	0.52
1:A:141:VAL:HG11	1:B:137:TYR:HB3	1.91	0.52
1:A:198:THR:O	1:A:201:VAL:HB	2.10	0.52
1:A:343:LEU:HD12	1:A:405:LEU:HD12	1.91	0.52
1:A:166:GLU:HB3	2:A:648:HOH:O	2.10	0.52
1:A:387:ASP:OD2	1:A:389:SER:HB2	2.10	0.52
1:A:360:LEU:HD11	2:B:457:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:GLY:O	1:A:429:PHE:HA	2.10	0.52
1:A:25:GLU:HG3	1:A:61:ARG:NH2	2.24	0.51
1:A:375:MET:CE	1:A:398:TYR:HA	2.40	0.51
1:A:267:LYS:HA	1:A:330:THR:OG1	2.10	0.51
1:A:31:VAL:HG22	1:A:67:ILE:HB	1.92	0.51
1:A:228:LEU:HB3	1:A:239:THR:HB	1.91	0.51
1:B:349:MET:HE1	1:B:368:VAL:HG22	1.92	0.51
1:A:2:ASN:ND2	2:A:534:HOH:O	2.44	0.51
1:A:349:MET:O	1:A:351:ASP:N	2.37	0.51
1:A:154:LYS:HD3	1:A:191:MET:CE	2.40	0.51
1:A:19:ILE:HD11	1:A:328:CYS:SG	2.51	0.51
1:B:80:MET:SD	1:B:193:VAL:HG11	2.50	0.51
1:B:322:ASN:O	1:B:323:SER:C	2.48	0.51
1:A:5:VAL:HG22	1:A:220:PHE:HB2	1.93	0.51
1:A:350:PRO:HG2	1:A:364:ASP:HB3	1.91	0.51
1:A:319:VAL:HA	1:A:324:LEU:HD12	1.93	0.51
1:A:164:VAL:HG11	2:A:488:HOH:O	2.10	0.51
1:A:309:TRP:NE1	1:A:342:LYS:HE3	2.24	0.50
1:A:118:GLU:HB3	1:A:119:LYS:HE3	1.92	0.50
1:A:191:MET:HE3	1:A:191:MET:HA	1.93	0.50
1:B:173:VAL:HG11	1:B:180:ALA:HB2	1.92	0.50
1:B:351:ASP:OD1	1:B:353:ARG:HB2	2.11	0.50
1:B:234:THR:O	1:B:237:TYR:N	2.44	0.50
1:B:426:ARG:O	1:B:427:ASP:HB3	2.11	0.50
1:B:59:ILE:O	1:B:96:ARG:NH2	2.36	0.50
1:B:70:ASN:HB2	1:B:102:ALA:HB3	1.94	0.50
1:A:154:LYS:HD3	1:A:191:MET:HE1	1.94	0.50
1:A:375:MET:HE1	1:A:398:TYR:HA	1.92	0.50
1:B:102:ALA:HA	1:B:147:ARG:HD2	1.93	0.50
1:B:32:ARG:HD3	2:B:476:HOH:O	2.12	0.50
1:A:138:GLU:HG3	1:B:138:GLU:HB3	1.93	0.50
1:A:114:ASP:O	1:A:118:GLU:HB2	2.12	0.50
1:A:151:LEU:HD22	1:A:194:ALA:HB2	1.94	0.50
1:A:403:GLU:O	1:A:407:GLY:N	2.42	0.49
1:A:267:LYS:HE3	1:A:271:THR:HG23	1.93	0.49
1:B:70:ASN:HB3	2:B:538:HOH:O	2.11	0.49
1:B:304:ARG:HG2	1:B:305:ARG:N	2.27	0.49
1:A:412:ILE:HA	1:A:423:MET:O	2.13	0.49
1:B:311:ASP:O	1:B:315:VAL:HG23	2.13	0.49
1:B:34:GLN:OE1	1:B:223:ALA:HB3	2.13	0.49
1:B:125:ALA:HA	2:B:640:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:LEU:HD21	1:B:309:TRP:CD1	2.48	0.49
1:B:50:THR:HG21	1:B:89:ARG:HH21	1.77	0.49
1:B:393:GLN:HE21	1:B:396:LEU:HB2	1.78	0.48
1:B:59:ILE:HD11	1:B:93:VAL:HA	1.96	0.48
1:B:77:ALA:HB1	2:B:460:HOH:O	2.13	0.48
1:A:22:LEU:O	1:A:25:GLU:HB2	2.14	0.48
1:B:128:THR:HG21	1:B:131:ARG:HE	1.78	0.48
1:A:16[A]:LYS:HG3	2:A:485:HOH:O	2.14	0.48
1:B:292:LYS:NZ	1:B:293:GLN:OE1	2.41	0.48
1:B:347:TYR:HB3	1:B:349:MET:HE2	1.94	0.48
1:B:21:ASP:HB3	1:B:419:ARG:NH2	2.28	0.48
1:B:239:THR:HG23	1:B:241:SER:H	1.79	0.48
1:B:244:THR:HB	1:B:322:ASN:OD1	2.14	0.48
1:A:317:ARG:HE	1:A:358:THR:HB	1.79	0.48
1:A:146:LEU:HD22	1:A:157:PHE:CD1	2.48	0.47
1:A:375:MET:HE1	1:A:397:ASN:O	2.14	0.47
1:A:267:LYS:HG2	1:A:269:TYR:O	2.14	0.47
1:B:338:LEU:O	1:B:377:GLY:HA3	2.13	0.47
1:B:68:ILE:HD12	1:B:99:LEU:HD22	1.96	0.47
1:A:303:ARG:HH11	1:A:303:ARG:HG3	1.79	0.47
1:A:295:ASN:HA	1:A:297:PHE:CE2	2.50	0.47
1:B:360:LEU:HD23	1:B:360:LEU:N	2.23	0.47
1:B:389:SER:HB3	2:B:496:HOH:O	2.13	0.47
1:A:289:PHE:CE2	1:A:338:LEU:HD21	2.49	0.47
1:A:289:PHE:CZ	1:A:293:GLN:NE2	2.83	0.47
1:B:131:ARG:HG3	1:B:131:ARG:HH11	1.80	0.47
1:B:332:LEU:O	1:B:334:VAL:N	2.48	0.47
1:B:1:GLY:N	1:B:431:ALA:O	2.40	0.46
1:A:118:GLU:CD	1:A:131:ARG:HH22	2.19	0.46
1:A:327:PHE:HB2	1:A:410:ILE:HA	1.96	0.46
1:A:262:VAL:HG12	1:A:324:LEU:HD23	1.96	0.46
1:B:91:ILE:O	1:B:93:VAL:HG23	2.15	0.46
1:A:239:THR:HG23	1:A:240:SER:N	2.31	0.46
1:B:316:ARG:NH1	2:B:570:HOH:O	2.43	0.46
1:A:20:VAL:HG22	1:A:219:MET:HE3	1.98	0.46
1:B:25:GLU:CD	1:B:419:ARG:HH11	2.19	0.46
1:B:256:PRO:O	1:B:259:VAL:HG23	2.16	0.46
1:B:412:ILE:HG12	1:B:424:ILE:HG12	1.97	0.46
1:B:32:ARG:HG2	1:B:56:PRO:HG3	1.98	0.46
1:A:155:GLU:O	1:A:158:ALA:HB3	2.16	0.46
1:A:228:LEU:O	1:A:238:VAL:CG2	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ASP:HB3	1:B:426:ARG:HB3	1.97	0.46
1:B:220:PHE:HZ	1:B:254:LEU:HD22	1.81	0.46
1:B:35:GLY:O	1:B:73:VAL:HG22	2.15	0.45
1:B:43:LEU:HD22	1:B:60:LEU:CD1	2.34	0.45
1:A:118:GLU:HB3	1:A:119:LYS:CE	2.46	0.45
1:A:391:LEU:HD12	1:A:396:LEU:HD12	1.99	0.45
1:A:61:ARG:NH2	2:A:474:HOH:O	2.46	0.45
1:B:345:VAL:HG12	1:B:405:LEU:HD11	1.97	0.45
1:A:366[A]:LYS:HG3	1:A:366[A]:LYS:O	2.17	0.45
1:A:278:PHE:CD2	1:A:306:ARG:HG3	2.51	0.45
1:B:1:GLY:HA2	1:B:260:ASP:HB3	1.99	0.45
1:B:132:GLY:HA2	1:B:135:PRO:HG2	1.99	0.45
1:B:332:LEU:C	1:B:334:VAL:H	2.21	0.45
1:B:130:GLY:HA3	1:B:133:ILE:HD11	1.99	0.45
1:B:132:GLY:O	1:B:133:ILE:C	2.55	0.45
1:B:268:ALA:O	1:B:310:LEU:HD23	2.18	0.44
1:A:191:MET:HE3	1:A:194:ALA:HB2	1.99	0.44
1:A:138:GLU:OE2	1:B:144:ARG:NH2	2.51	0.44
1:B:331:LYS:NZ	2:B:618:HOH:O	2.48	0.44
1:A:151:LEU:HD22	1:A:194:ALA:CB	2.48	0.44
1:B:347:TYR:O	1:B:354:GLU:HA	2.17	0.44
1:A:84:LYS:HE2	1:A:84:LYS:HA	2.00	0.44
1:A:413:ILE:HB	1:A:423:MET:HB2	1.99	0.44
1:A:383:PHE:CZ	1:A:417:PRO:HD2	2.53	0.44
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.57	0.44
1:A:182:ASP:HA	2:A:583:HOH:O	2.17	0.44
1:B:426:ARG:NH1	2:B:540:HOH:O	2.51	0.43
1:A:101:GLU:HG2	1:B:360:LEU:HD12	2.00	0.43
1:B:292:LYS:HE2	1:B:292:LYS:HB2	1.78	0.43
1:A:129:THR:O	1:A:130:GLY:O	2.36	0.43
1:B:261:TYR:HE1	1:B:263:LEU:HB2	1.83	0.43
1:A:280:THR:CG2	1:A:309:TRP:O	2.64	0.43
1:B:101:GLU:OE1	1:B:147:ARG:NH2	2.49	0.43
1:A:42:THR:C	1:A:43:LEU:HD12	2.39	0.43
1:A:303:ARG:HG3	1:A:303:ARG:NH1	2.32	0.43
1:A:143:ARG:HD3	1:B:238:VAL:HG23	2.01	0.43
1:A:361:ALA:N	1:B:101:GLU:OE2	2.41	0.43
1:A:357:THR:O	1:A:358:THR:C	2.57	0.43
1:B:170:PHE:O	1:B:174:ASN:HB2	2.18	0.43
1:B:345:VAL:HG12	1:B:405:LEU:CD1	2.48	0.43
1:B:128:THR:CG2	1:B:131:ARG:NE	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:VAL:HG11	1:A:391:LEU:HD23	2.00	0.43
1:A:176:TYR:O	1:A:177:LYS:HB2	2.18	0.43
1:B:361:ALA:O	1:B:365:TRP:HD1	2.02	0.43
1:A:20:VAL:HG13	1:A:219:MET:CE	2.49	0.43
1:B:333:ASP:N	1:B:333:ASP:OD1	2.52	0.43
1:A:143:ARG:NH1	1:B:238:VAL:O	2.52	0.42
1:A:97:LEU:HB3	1:A:200:MET:HE1	1.98	0.42
1:A:366[A]:LYS:HA	2:A:454:HOH:O	2.19	0.42
1:B:64:VAL:HG12	1:B:65:THR:N	2.33	0.42
1:A:138:GLU:OE1	1:B:142:ALA:HB2	2.19	0.42
1:A:236:PRO:O	1:A:238:VAL:HG12	2.19	0.42
1:A:333:ASP:OD2	1:A:383:PHE:HD2	2.02	0.42
1:A:232:HIS:CE1	1:B:253:GLY:CA	3.02	0.42
1:B:27:ALA:O	1:B:64:VAL:HG22	2.19	0.42
1:B:332:LEU:C	1:B:334:VAL:N	2.73	0.42
1:A:366[B]:LYS:O	1:A:366[B]:LYS:HG2	2.20	0.42
1:A:225:GLY:O	1:A:228:LEU:HB2	2.19	0.42
1:A:37:HIS:CE1	1:A:130:GLY:O	2.73	0.42
1:B:370:PRO:HG2	1:B:372:TYR:CE2	2.54	0.42
1:B:83:MET:CE	1:B:94:ARG:HG2	2.49	0.42
1:A:388:ARG:O	1:A:391:LEU:HB2	2.19	0.42
1:A:347:TYR:HB3	1:A:368:VAL:CG2	2.49	0.42
1:A:245:ALA:O	1:A:248:VAL:HG23	2.18	0.42
1:B:427:ASP:HA	1:B:428:PRO:HD3	1.78	0.42
1:A:220:PHE:CZ	1:A:254:LEU:HD22	2.55	0.42
1:A:68:ILE:HG23	1:A:72:VAL:HG21	2.02	0.42
1:A:24:THR:HG23	1:A:30:VAL:HG21	2.02	0.42
1:A:319:VAL:HG22	1:A:324:LEU:HD12	2.02	0.41
1:B:25:GLU:CD	1:B:419:ARG:NH1	2.74	0.41
1:B:25:GLU:OE2	1:B:419:ARG:NH1	2.53	0.41
1:A:309:TRP:CE2	1:A:342:LYS:HG3	2.56	0.41
1:B:402:ILE:O	1:B:406:THR:HG23	2.20	0.41
1:A:101:GLU:HG2	1:B:360:LEU:CD1	2.51	0.41
1:B:370:PRO:CG	1:B:372:TYR:CE2	3.03	0.41
1:B:227:LEU:O	1:B:233:GLY:HA3	2.21	0.41
1:A:109:TYR:O	1:A:113:LEU:HD22	2.20	0.41
1:B:162:LYS:HE3	1:B:183:TYR:CZ	2.56	0.41
1:B:185[A]:LYS:HB3	1:B:185[A]:LYS:HE3	1.84	0.41
1:A:118:GLU:CB	1:A:119:LYS:NZ	2.84	0.41
1:A:349:MET:HB2	1:A:351:ASP:OD1	2.20	0.41
1:B:269:TYR:CD1	1:B:269:TYR:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ARG:HD3	1:A:431:ALA:HB2	2.03	0.41
1:B:6:VAL:HG13	1:B:265:ILE:HD11	2.03	0.41
1:B:101:GLU:O	1:B:147:ARG:HB3	2.20	0.41
1:A:366[B]:LYS:HA	2:A:454:HOH:O	2.20	0.41
1:B:19:ILE:HD13	1:B:265:ILE:HD12	2.03	0.41
1:A:23:LEU:C	1:A:25:GLU:H	2.24	0.41
1:B:386:LYS:HE2	1:B:420:THR:C	2.41	0.41
1:A:19:ILE:CG1	1:A:328:CYS:SG	3.09	0.41
1:A:413:ILE:HG22	1:A:413:ILE:O	2.21	0.41
1:A:346:ALA:HB3	1:A:371:ILE:HB	2.02	0.41
1:A:107:LEU:HD22	2:A:548:HOH:O	2.21	0.41
1:B:396:LEU:HD23	1:B:396:LEU:HA	1.81	0.41
1:B:276:GLY:O	1:B:306:ARG:NH2	2.47	0.41
1:A:10:GLN:HG2	2:A:472:HOH:O	2.20	0.41
1:A:228:LEU:O	1:A:238:VAL:HG22	2.20	0.40
1:B:278:PHE:CD2	1:B:281:GLU:HB2	2.56	0.40
1:B:109:TYR:HD2	1:B:168:HIS:CD2	2.38	0.40
1:B:267:LYS:HE3	1:B:271:THR:HG23	2.02	0.40
1:B:101:GLU:HG3	1:B:147:ARG:HH12	1.85	0.40
1:B:172:LEU:HD23	1:B:172:LEU:HA	1.82	0.40
1:B:202:VAL:CG1	1:B:203:ASP:N	2.84	0.40
1:B:282:LEU:HD21	1:B:309:TRP:NE1	2.37	0.40
1:A:290:LEU:HD23	1:A:290:LEU:HA	1.95	0.40
1:A:229:ASP:OD2	1:A:244:THR:HG23	2.22	0.40
1:A:14:GLU:HB2	2:A:517:HOH:O	2.21	0.40

All (1) 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:B:348:ARG:HH21	1:B:430:ASP:OD2[4_555]	1.53	0.07

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	436/431 (101%)	374 (86%)	49 (11%)	13 (3%)	5	7
1	B	433/431 (100%)	391 (90%)	33 (8%)	9 (2%)	9	14
All	All	869/862 (101%)	765 (88%)	82 (9%)	22 (2%)	7	10

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	ASP
1	B	131	ARG
1	A	123	ALA
1	A	128	THR
1	A	145	GLY
1	A	304	ARG
1	A	383	PHE
1	A	131	ARG
1	A	268	ALA
1	A	301	THR
1	B	127	GLY
1	B	333	ASP
1	A	24	THR
1	A	130	GLY
1	A	427	ASP
1	B	303	ARG
1	B	427	ASP
1	B	122	GLY
1	B	133	ILE
1	A	368	VAL
1	B	92	PRO
1	B	278	PHE

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	360/353 (102%)	325 (90%)	35 (10%)	10	19
1	B	357/353 (101%)	323 (90%)	34 (10%)	11	20
All	All	717/706 (102%)	648 (90%)	69 (10%)	10	19

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	37	HIS
1	A	42	THR
1	A	46	ASN
1	A	63	ASN
1	A	73	VAL
1	A	84	LYS
1	A	99	LEU
1	A	101	GLU
1	A	113	LEU
1	A	114	ASP
1	A	119	LYS
1	A	121	ARG
1	A	129	THR
1	A	131	ARG
1	A	143	ARG
1	A	191	MET
1	A	201	VAL
1	A	202	VAL
1	A	207	LEU
1	A	239	THR
1	A	270	SER
1	A	280	THR
1	A	300	THR
1	A	301	THR
1	A	303	ARG
1	A	306	ARG
1	A	343	LEU
1	A	356	THR
1	A	379	SER
1	A	387	ASP
1	A	391	LEU
1	A	397	ASN
1	A	401	ARG
1	A	426	ARG

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Mol	Chain	Res	Type
1	B	7	LEU
1	B	18	LYS
1	B	34	GLN
1	B	51	VAL
1	B	61	ARG
1	B	73	VAL
1	B	74	LEU
1	B	76	PRO
1	B	81	LYS
1	B	82	GLU
1	B	114	ASP
1	B	115	ASN
1	B	118	GLU
1	B	133	ILE
1	B	141	VAL
1	B	143	ARG
1	B	144	ARG
1	B	166	GLU
1	B	185[A]	LYS
1	B	185[B]	LYS
1	B	213	GLN
1	B	224	GLN
1	B	230	ILE
1	B	231	ASP
1	B	285	GLU
1	B	288	GLU
1	B	310	LEU
1	B	350	PRO
1	B	360	LEU
1	B	379	SER
1	B	391	LEU
1	B	422	THR
1	B	426	ARG
1	B	430	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	168	HIS
1	A	224	GLN
1	B	2	ASN

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Mol	Chain	Res	Type
1	B	171	GLN
1	B	210	GLN
1	B	224	GLN
1	B	242	ASN
1	B	393	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.