



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:18 PM UTC

PDB ID : 3DRD / pdb\_00003drd  
Title : Crystal Structure of 7,8 Diaminopelargonic Acid Synthase Apoenzyme in Bacillus subtilis  
Authors : Dey, S.; Sacchettini, J.C.  
Deposited on : 2008-07-11  
Resolution : 2.17 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
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

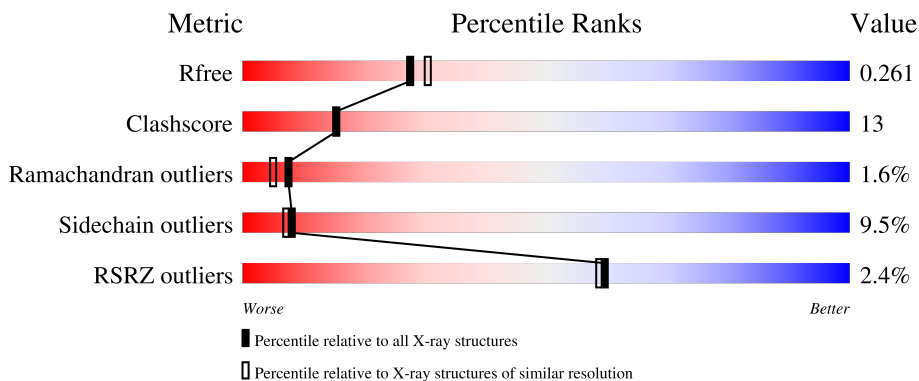
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.17 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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  $\geq 3$ , 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	448	 2% 65% 23% 6%
1	B	448	 2% 67% 21% 5% 7%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6826 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 Adenosylmethionine-8-amino-7-oxononanoate aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	419	3296	2102	546	625	23	0	0	0
1	B	417	3280	2093	544	621	22	0	0	0

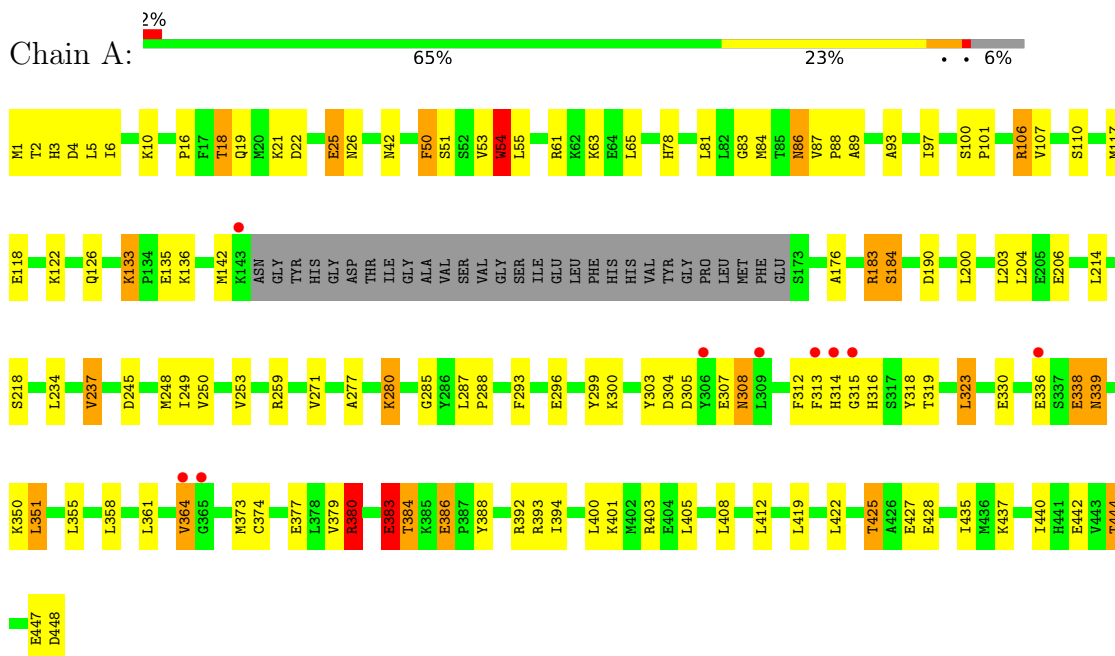
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	121	121	121	0	0
2	B	129	129	129	0	0

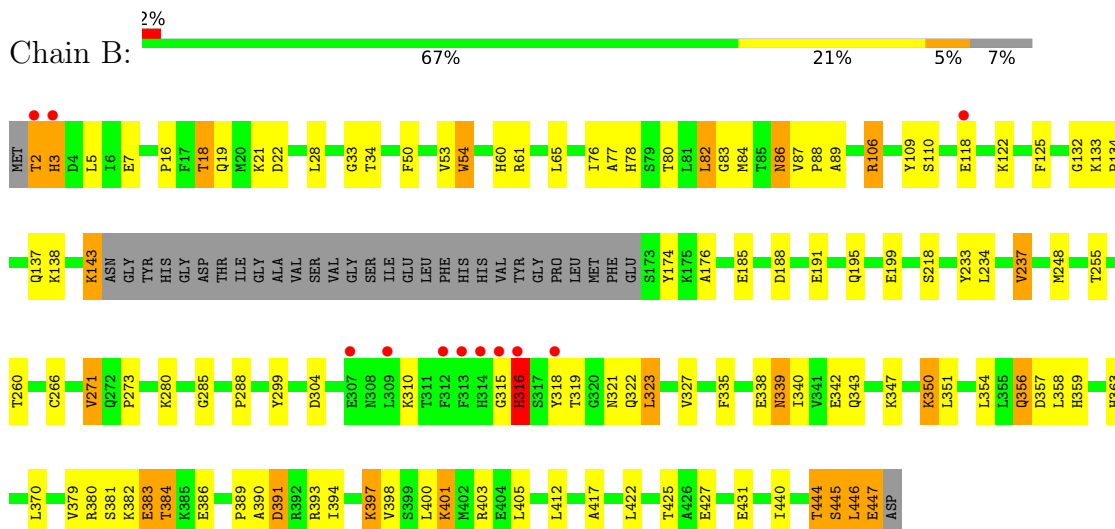
### 3 Residue-property plots

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: Adenosylmethionine-8-amino-7-oxononanoate aminotransferase



- Molecule 1: Adenosylmethionine-8-amino-7-oxononanoate aminotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.17Å 102.84Å 74.56Å 90.00° 105.15° 90.00°	Depositor
Resolution (Å)	35.00 – 2.17 35.00 – 2.17	Depositor EDS
% Data completeness (in resolution range)	93.0 (35.00-2.17) 93.0 (35.00-2.17)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.33 (at 2.18Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.205 , 0.265 0.202 , 0.261	Depositor DCC
$R_{free}$ test set	2098 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtrriage
Anisotropy	0.304	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 36.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6826	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.58	0/3363	0.94	8/4536 (0.2%)
1	B	0.59	0/3347	0.90	2/4515 (0.0%)
All	All	0.58	0/6710	0.92	10/9051 (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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	384	THR	N-CA-C	-10.34	101.16	113.88
1	B	3	HIS	N-CA-C	-10.08	100.85	113.55
1	B	316	HIS	N-CA-C	6.37	117.02	108.23
1	A	54	TRP	N-CA-C	6.19	119.71	111.30
1	A	133	LYS	CA-C-N	6.18	126.98	120.12
1	A	133	LYS	C-N-CA	6.18	126.98	120.12
1	A	383	GLU	N-CA-C	5.62	122.77	110.80
1	A	380	ARG	N-CA-CB	5.15	118.24	110.30
1	A	442	GLU	N-CA-C	5.11	116.54	111.07
1	A	190	ASP	N-CA-C	5.09	116.52	111.07

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	ARG	Peptide
1	A	383	GLU	Peptide
1	B	390	ALA	Peptide

## 5.2 Too-close contacts [i](#)

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	3296	0	3292	97	0
1	B	3280	0	3276	93	0
2	A	121	0	0	3	0
2	B	129	0	0	6	0
All	All	6826	0	6568	177	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 13.

All (177) 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:117:MET:HE3	1:A:277:ALA:CB	1.92	1.00
1:B:188:ASP:OD1	1:B:191:GLU:HG3	1.65	0.97
1:A:350:LYS:HD3	2:A:630:HOH:O	1.65	0.97
1:A:117:MET:HE3	1:A:277:ALA:HB3	1.49	0.93
1:A:447:GLU:O	1:A:448:ASP:HB2	1.71	0.90
1:A:2:THR:O	1:A:6:ILE:HG13	1.71	0.90
1:B:440:ILE:O	1:B:444:THR:HB	1.74	0.86
1:B:393:ARG:O	1:B:397:LYS:HG2	1.77	0.84
1:A:383:GLU:O	1:A:383:GLU:HG2	1.78	0.82
1:B:350:LYS:H	1:B:350:LYS:HD2	1.44	0.80
1:A:19:GLN:HE21	1:A:21:LYS:H	1.28	0.79
1:B:77:ALA:HA	1:B:323:LEU:HD13	1.66	0.77
1:B:80:THR:HG22	1:B:84:MET:HE2	1.68	0.76
1:A:117:MET:HE3	1:A:277:ALA:HB2	1.67	0.74
1:B:110:SER:HB2	1:B:316:HIS:HE1	1.52	0.74
1:B:28:LEU:HD22	1:B:403:ARG:HD2	1.70	0.74
1:B:16:PRO:O	1:B:18:THR:CG2	2.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:MET:CE	1:A:277:ALA:HB2	2.18	0.73
1:B:19:GLN:HE21	1:B:21:LYS:H	1.37	0.71
1:B:134:PRO:HG3	2:B:686:HOH:O	1.91	0.71
1:A:106:ARG:HG2	1:A:299:TYR:CD1	2.26	0.70
1:B:350:LYS:HD2	1:B:350:LYS:N	2.08	0.69
1:B:363:HIS:HB2	1:B:444:THR:HG21	1.75	0.69
1:A:83:GLY:H	1:B:18:THR:HG21	1.57	0.68
1:A:118:GLU:O	1:A:122:LYS:HG2	1.93	0.68
1:B:381:SER:OG	1:B:384:THR:HG21	1.94	0.68
1:B:16:PRO:O	1:B:18:THR:HG22	1.92	0.68
1:A:425:THR:HG22	1:A:428:GLU:H	1.59	0.68
1:B:2:THR:OG1	1:B:3:HIS:N	2.26	0.67
1:B:86:ASN:ND2	1:B:89:ALA:H	1.92	0.67
1:B:383:GLU:H	1:B:383:GLU:CD	2.04	0.66
1:A:308:ASN:N	1:A:308:ASN:OD1	2.26	0.66
1:B:188:ASP:OD1	1:B:191:GLU:CG	2.43	0.65
1:A:87:VAL:HB	1:A:88:PRO:HD3	1.78	0.65
1:A:16:PRO:HG2	1:B:82:LEU:HD22	1.77	0.65
1:A:19:GLN:NE2	1:A:21:LYS:H	1.95	0.64
1:A:307:GLU:HG2	1:A:308:ASN:OD1	1.97	0.64
1:A:18:THR:HG21	1:B:83:GLY:H	1.62	0.63
1:A:383:GLU:O	1:A:383:GLU:CG	2.46	0.63
1:A:384:THR:OG1	1:A:386:GLU:HG2	1.99	0.62
1:B:444:THR:C	1:B:446:LEU:H	2.07	0.62
1:A:447:GLU:O	1:A:448:ASP:CB	2.49	0.59
1:A:26:ASN:O	1:A:403:ARG:NH2	2.35	0.59
1:A:16:PRO:O	1:A:18:THR:HG22	2.02	0.59
1:B:389:PRO:HB2	1:B:391:ASP:HB2	1.86	0.58
1:A:315:GLY:HA3	1:B:16:PRO:HB3	1.85	0.58
1:A:1:MET:HG3	1:A:3:HIS:H	1.68	0.58
1:B:2:THR:N	1:B:5:LEU:HD12	2.17	0.58
1:B:384:THR:OG1	1:B:386:GLU:HB2	2.04	0.58
1:B:304:ASP:HB2	1:B:310:LYS:HE2	1.87	0.57
1:A:86:ASN:HD22	1:A:88:PRO:HD2	1.69	0.57
1:B:381:SER:OG	1:B:384:THR:CG2	2.51	0.57
1:A:440:ILE:O	1:A:444:THR:HB	2.04	0.57
1:A:142:MET:SD	1:A:176:ALA:HB3	2.45	0.57
1:A:93:ALA:O	1:A:97:ILE:HG12	2.05	0.56
1:B:427:GLU:O	1:B:431:GLU:HG3	2.06	0.56
1:A:316:HIS:HB2	1:A:319:THR:HG23	1.88	0.56
1:A:315:GLY:HA3	1:B:16:PRO:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HG3	1:A:2:THR:N	2.21	0.55
1:B:110:SER:CB	1:B:316:HIS:HE1	2.17	0.55
1:B:16:PRO:O	1:B:18:THR:HG23	2.05	0.55
1:B:110:SER:HB2	1:B:316:HIS:CE1	2.38	0.55
1:B:33:GLY:O	1:B:61:ARG:HD3	2.06	0.55
1:A:133:LYS:HB2	1:A:135:GLU:OE1	2.07	0.55
1:B:248:MET:CE	1:B:273:PRO:HA	2.38	0.54
1:B:389:PRO:HB2	1:B:391:ASP:CB	2.37	0.54
1:B:54:TRP:CD1	1:B:54:TRP:N	2.74	0.54
1:A:380:ARG:HB3	1:A:388:TYR:CE2	2.42	0.54
1:A:1:MET:HB3	1:A:4:ASP:OD2	2.08	0.54
1:B:425:THR:OG1	1:B:427:GLU:HG2	2.08	0.54
1:B:401:LYS:HE3	1:B:401:LYS:HA	1.88	0.54
1:A:307:GLU:CG	1:A:308:ASN:OD1	2.56	0.53
1:A:285:GLY:HA2	1:B:318:TYR:OH	2.09	0.53
1:A:21:LYS:O	1:A:25:GLU:HG2	2.09	0.53
1:A:50:PHE:HD2	1:A:50:PHE:H	1.57	0.52
1:A:373:MET:HG3	1:A:419:LEU:HD21	1.90	0.52
1:B:86:ASN:HD21	1:B:89:ALA:H	1.57	0.52
1:A:237:VAL:HG22	1:A:248:MET:HE3	1.92	0.52
1:B:363:HIS:ND1	1:B:444:THR:HG23	2.23	0.52
1:B:87:VAL:HB	1:B:88:PRO:HD3	1.92	0.51
1:A:351:LEU:HD22	1:A:355:LEU:HG	1.91	0.51
1:A:136:LYS:NZ	1:A:245:ASP:O	2.43	0.51
1:A:16:PRO:O	1:A:18:THR:CG2	2.60	0.49
1:B:393:ARG:HD2	2:B:693:HOH:O	2.12	0.49
1:A:22:ASP:CG	1:A:393:ARG:HH22	2.21	0.49
1:A:259:ARG:HD2	1:A:419:LEU:HD23	1.95	0.49
1:B:106:ARG:HG2	1:B:299:TYR:CD1	2.48	0.49
1:B:118:GLU:O	1:B:122:LYS:HG3	2.13	0.49
1:A:380:ARG:HD2	1:A:386:GLU:OE2	2.13	0.49
1:B:260:THR:HB	1:B:370:LEU:HG	1.94	0.49
1:A:313:PHE:O	1:A:314:HIS:CG	2.66	0.48
1:A:18:THR:HG21	1:B:83:GLY:N	2.28	0.48
1:A:117:MET:HE2	1:A:277:ALA:HB2	1.93	0.48
1:B:444:THR:C	1:B:446:LEU:N	2.72	0.48
1:A:361:LEU:HB2	1:A:364:VAL:HG23	1.95	0.48
1:B:394:ILE:O	1:B:398:VAL:HG23	2.14	0.48
1:A:405:LEU:HB3	1:A:435:ILE:HG23	1.96	0.48
1:B:195:GLN:O	1:B:199:GLU:HG3	2.13	0.48
1:A:338:GLU:O	1:A:339:ASN:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:GLN:O	1:B:359:HIS:HB2	2.14	0.47
1:B:248:MET:HE2	1:B:273:PRO:HA	1.95	0.47
1:B:315:GLY:HA2	2:B:514:HOH:O	2.14	0.47
1:A:303:TYR:HA	1:B:19:GLN:HE22	1.80	0.47
1:B:34:THR:HG22	1:B:61:ARG:NH2	2.29	0.47
1:A:296:GLU:O	1:A:300:LYS:HG2	2.15	0.47
1:B:133:LYS:N	1:B:134:PRO:HD3	2.30	0.47
1:A:16:PRO:CG	1:B:82:LEU:HD22	2.42	0.47
1:A:133:LYS:HG3	1:A:136:LYS:HG3	1.96	0.47
1:B:82:LEU:N	1:B:82:LEU:HD23	2.30	0.46
1:A:318:TYR:OH	1:B:285:GLY:HA2	2.16	0.46
1:B:363:HIS:HB2	1:B:444:THR:CG2	2.44	0.46
1:B:446:LEU:O	1:B:447:GLU:C	2.58	0.46
1:A:86:ASN:ND2	1:A:88:PRO:HD2	2.31	0.46
1:B:444:THR:HG22	1:B:445:SER:N	2.30	0.46
1:B:412:LEU:CD2	1:B:417:ALA:HB2	2.46	0.46
1:A:118:GLU:HG2	1:A:122:LYS:HE3	1.98	0.45
1:B:359:HIS:O	1:B:382:LYS:NZ	2.49	0.45
1:B:132:GLY:C	1:B:134:PRO:HD3	2.42	0.45
1:B:233:TYR:O	1:B:237:VAL:HG12	2.16	0.45
1:B:422:LEU:HD12	1:B:422:LEU:N	2.31	0.45
1:A:392:ARG:NH2	1:A:447:GLU:OE2	2.48	0.45
1:A:117:MET:CE	1:A:277:ALA:CB	2.72	0.45
1:A:218:SER:HB2	1:A:250:VAL:CG1	2.46	0.45
1:A:50:PHE:N	1:A:50:PHE:CD2	2.85	0.45
1:A:408:LEU:HD13	1:B:84:MET:HE1	1.99	0.45
1:A:330:GLU:HA	1:A:330:GLU:OE2	2.17	0.45
1:A:361:LEU:HD11	1:A:437:LYS:HG3	1.99	0.45
1:B:125:PHE:CE1	1:B:137:GLN:HB2	2.52	0.45
1:B:393:ARG:CD	2:B:693:HOH:O	2.65	0.45
1:A:287:LEU:HD23	1:B:321:ASN:HD21	1.83	0.44
1:A:117:MET:HE1	1:A:249:ILE:CG2	2.47	0.44
1:B:22:ASP:CG	1:B:393:ARG:HH22	2.25	0.44
1:B:65:LEU:HG	1:B:327:VAL:HG22	1.99	0.44
1:A:51:SER:HB2	1:A:54:TRP:HA	2.00	0.44
1:B:339:ASN:O	1:B:343:GLN:HG2	2.18	0.44
1:B:384:THR:C	1:B:386:GLU:H	2.25	0.44
1:A:126:GLN:HE22	1:A:312:PHE:HA	1.83	0.44
1:A:86:ASN:ND2	1:A:89:ALA:H	2.16	0.43
1:B:384:THR:C	1:B:386:GLU:N	2.75	0.43
2:A:555:HOH:O	1:B:60:HIS:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:SER:O	1:B:255:THR:HG21	2.18	0.43
1:B:354:LEU:HD22	2:B:696:HOH:O	2.17	0.43
1:A:78:HIS:CE1	1:A:318:TYR:HA	2.53	0.43
1:A:97:ILE:HD11	1:A:107:VAL:HG23	2.01	0.42
1:B:380:ARG:NH2	1:B:389:PRO:HD3	2.35	0.42
1:B:335:PHE:HA	1:B:340:ILE:HG12	1.99	0.42
1:A:358:LEU:O	1:A:364:VAL:HG21	2.19	0.42
1:A:401:LYS:O	1:A:405:LEU:HD23	2.19	0.42
1:A:425:THR:HG22	1:A:427:GLU:N	2.34	0.42
1:A:81:LEU:HA	1:A:84:MET:O	2.19	0.42
1:B:397:LYS:HG2	1:B:397:LYS:H	1.63	0.42
1:B:18:THR:HB	2:B:748:HOH:O	2.19	0.42
1:A:364:VAL:O	1:A:379:VAL:HG22	2.20	0.42
1:B:266:CYS:HB2	1:B:271:VAL:HG22	2.02	0.42
1:A:117:MET:HE2	1:A:117:MET:HA	2.01	0.42
1:A:110:SER:HA	1:A:319:THR:HG22	2.02	0.41
1:A:305:ASP:HB2	1:A:308:ASN:OD1	2.19	0.41
1:B:78:HIS:HA	1:B:322:GLN:OE1	2.20	0.41
1:B:109:TYR:HB2	1:B:319:THR:HG23	2.01	0.41
1:A:288:PRO:HG2	1:B:288:PRO:HG2	2.01	0.41
1:A:323:LEU:HD12	1:A:323:LEU:HA	1.85	0.41
1:A:425:THR:CG2	1:A:427:GLU:H	2.34	0.41
1:B:422:LEU:N	1:B:422:LEU:CD1	2.84	0.41
1:A:22:ASP:OD2	1:A:393:ARG:NH2	2.54	0.41
1:A:100:SER:O	1:A:101:PRO:C	2.61	0.41
1:B:138:LYS:HD3	1:B:174:TYR:CE1	2.56	0.41
1:A:122:LYS:NZ	1:A:314:HIS:CD2	2.89	0.41
1:A:203:LEU:O	1:A:203:LEU:HD23	2.20	0.41
1:B:143:LYS:HD3	1:B:176:ALA:O	2.21	0.41
1:A:364:VAL:O	1:A:377:GLU:O	2.39	0.41
1:A:444:THR:CG2	2:A:563:HOH:O	2.69	0.40
1:B:110:SER:CB	1:B:316:HIS:CE1	3.02	0.40
1:A:2:THR:HG21	1:A:42:ASN:ND2	2.36	0.40
1:A:106:ARG:O	1:A:293:PHE:HA	2.21	0.40
1:A:253:VAL:O	1:A:280:LYS:HD2	2.21	0.40
1:A:380:ARG:HB3	1:A:388:TYR:CD2	2.56	0.40
1:A:214:LEU:HD23	1:A:214:LEU:C	2.46	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	415/448 (93%)	393 (95%)	15 (4%)	7 (2%)	7	4
1	B	413/448 (92%)	394 (95%)	13 (3%)	6 (2%)	8	5
All	All	828/896 (92%)	787 (95%)	28 (3%)	13 (2%)	7	5

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	383	GLU
1	B	391	ASP
1	A	339	ASN
1	A	364	VAL
1	B	445	SER
1	A	184	SER
1	A	280	LYS
1	A	304	ASP
1	B	280	LYS
1	B	339	ASN
1	A	53	VAL
1	B	76	ILE
1	B	53	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	355/378 (94%)	321 (90%)	34 (10%)	8	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	353/378 (93%)	320 (91%)	33 (9%)	8	7
All	All	708/756 (94%)	641 (90%)	67 (10%)	8	7

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	10	LYS
1	A	18	THR
1	A	25	GLU
1	A	50	PHE
1	A	54	TRP
1	A	55	LEU
1	A	61	ARG
1	A	63	LYS
1	A	65	LEU
1	A	86	ASN
1	A	106	ARG
1	A	183	ARG
1	A	184	SER
1	A	200	LEU
1	A	204	LEU
1	A	206	GLU
1	A	234	LEU
1	A	237	VAL
1	A	271	VAL
1	A	308	ASN
1	A	323	LEU
1	A	336	GLU
1	A	338	GLU
1	A	351	LEU
1	A	374	CYS
1	A	380	ARG
1	A	386	GLU
1	A	394	ILE
1	A	400	LEU
1	A	412	LEU
1	A	422	LEU
1	A	425	THR
1	A	444	THR
1	B	2	THR
1	B	7	GLU

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Mol	Chain	Res	Type
1	B	18	THR
1	B	50	PHE
1	B	54	TRP
1	B	82	LEU
1	B	86	ASN
1	B	106	ARG
1	B	143	LYS
1	B	185	GLU
1	B	234	LEU
1	B	237	VAL
1	B	271	VAL
1	B	316	HIS
1	B	323	LEU
1	B	338	GLU
1	B	342	GLU
1	B	347	LYS
1	B	350	LYS
1	B	351	LEU
1	B	356	GLN
1	B	357	ASP
1	B	358	LEU
1	B	379	VAL
1	B	383	GLU
1	B	384	THR
1	B	397	LYS
1	B	400	LEU
1	B	401	LYS
1	B	405	LEU
1	B	444	THR
1	B	446	LEU
1	B	447	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	42	ASN
1	A	60	HIS
1	A	72	GLN
1	A	86	ASN
1	A	91	GLN
1	A	126	GLN

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Mol	Chain	Res	Type
1	A	137	GLN
1	A	207	HIS
1	A	221	GLN
1	A	314	HIS
1	A	343	GLN
1	A	359	HIS
1	B	19	GLN
1	B	60	HIS
1	B	86	ASN
1	B	91	GLN
1	B	195	GLN
1	B	207	HIS
1	B	316	HIS
1	B	321	ASN
1	B	331	ASN
1	B	343	GLN
1	B	359	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](#)

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	419/448 (93%)	0.08	9 (2%) 63 63	14, 26, 44, 60	1 (0%)
1	B	417/448 (93%)	-0.00	11 (2%) 57 56	12, 25, 41, 61	1 (0%)
All	All	836/896 (93%)	0.04	20 (2%) 59 59	12, 25, 42, 61	2 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	313	PHE	7.6
1	B	2	THR	4.6
1	A	314	HIS	4.1
1	B	3	HIS	4.0
1	B	313	PHE	3.9
1	B	315	GLY	3.3
1	B	314	HIS	3.2
1	B	316	HIS	3.1
1	B	309	LEU	2.9
1	A	336	GLU	2.8
1	A	309	LEU	2.4
1	A	315	GLY	2.4
1	A	306	TYR	2.4
1	A	365	GLY	2.3
1	A	364	VAL	2.3
1	B	312	PHE	2.2
1	B	118	GLU	2.1
1	B	318	TYR	2.1
1	A	143	LYS	2.1
1	B	307	GLU	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.