



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2025 – 12:07 pm GMT

PDB ID : 9H3I  
Title : trans-aconitate decarboxylase Tad1- wild type  
Authors : Zheng, L.; Bang, G.  
Deposited on : 2024-10-16  
Resolution : 2.31 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 : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41

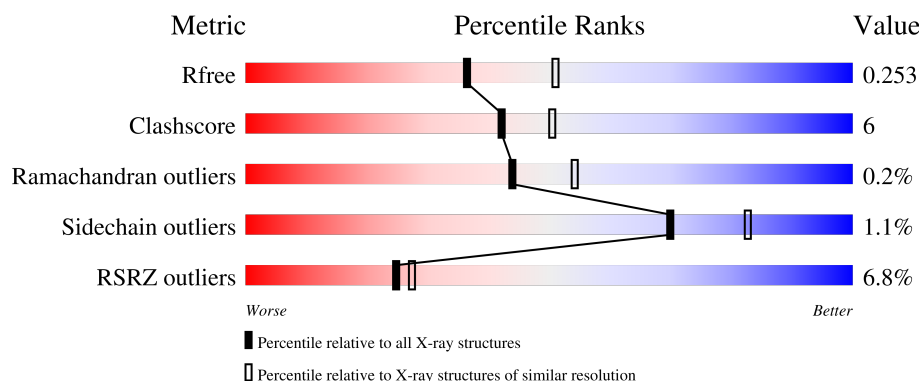
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 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))
$R_{free}$	164625	7250 (2.34-2.30)
Clashscore	180529	8063 (2.34-2.30)
Ramachandran outliers	177936	7993 (2.34-2.30)
Sidechain outliers	177891	7993 (2.34-2.30)
RSRZ outliers	164620	7250 (2.34-2.30)

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	493	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>15%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	493	<div> <div>12%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>•</div> <div>12%</div> </div> </div>
1	C	493	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	493	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>•</div> <div>11%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13546 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 Trans-aconitate decarboxylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	437	Total	C	N	O	S	0	0	0
			3379	2126	596	635	22			
1	A	436	Total	C	N	O	S	0	0	0
			3368	2124	593	629	22			
1	B	434	Total	C	N	O	S	0	0	0
			3361	2117	592	630	22			
1	C	439	Total	C	N	O	S	0	0	0
			3384	2132	595	635	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	489	PRO	ARG	conflict	UNP A0A0U2UYC4
A	489	PRO	ARG	conflict	UNP A0A0U2UYC4
B	489	PRO	ARG	conflict	UNP A0A0U2UYC4
C	489	PRO	ARG	conflict	UNP A0A0U2UYC4

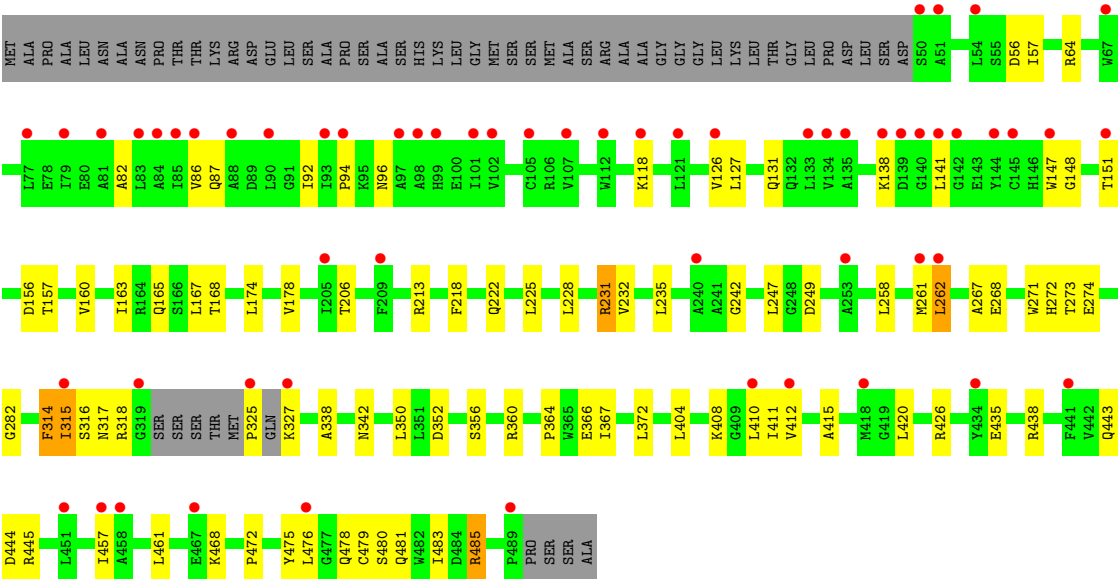
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	21	Total	O	0	0
			21	21		
2	A	16	Total	O	0	0
			16	16		
2	B	4	Total	O	0	0
			4	4		
2	C	13	Total	O	0	0
			13	13		

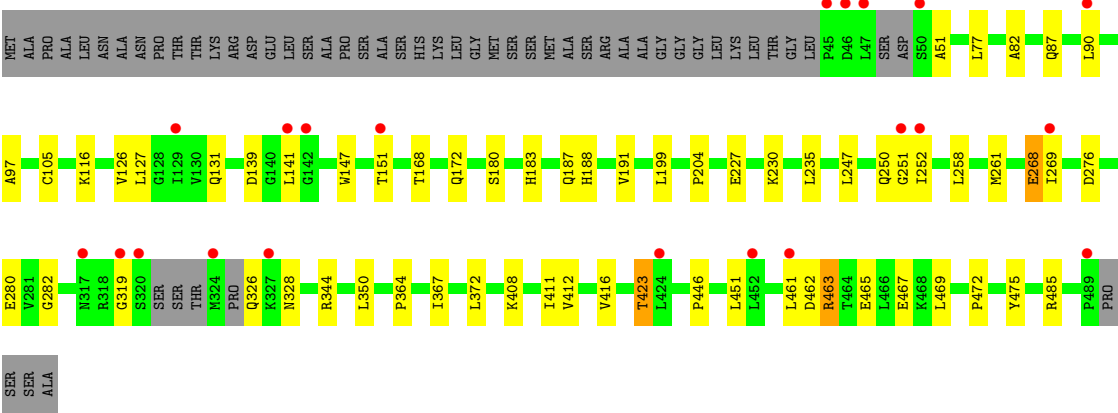
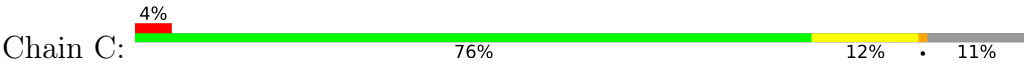


- Molecule 1: Trans-aconitate decarboxylase 1





• Molecule 1: Trans-aconitase decarboxylase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.62Å 164.69Å 208.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 2.31 49.72 – 2.31	Depositor EDS
% Data completeness (in resolution range)	97.7 (49.72-2.31) 97.8 (49.72-2.31)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.227 , 0.257 0.225 , 0.253	Depositor DCC
$R_{free}$ test set	8322 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.1	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13546	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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

### 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	0.33	0/3430	0.55	1/4656 (0.0%)
1	B	0.30	0/3424	0.55	0/4648
1	C	0.31	0/3447	0.53	0/4680
1	D	0.31	0/3442	0.55	0/4672
All	All	0.31	0/13743	0.55	1/18656 (0.0%)

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	D	0	2
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	467	GLU	CA-CB-CG	5.62	125.76	113.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	GLU	Peptide
1	A	467	GLU	Peptide
1	D	426	ARG	Sidechain
1	D	463	ARG	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	3368	0	3329	46	2
1	B	3361	0	3324	60	0
1	C	3384	0	3334	41	2
1	D	3379	0	3337	37	0
2	A	16	0	0	1	0
2	B	4	0	0	1	0
2	C	13	0	0	1	0
2	D	21	0	0	0	0
All	All	13546	0	13324	167	2

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 6.

All (167) 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:338:ALA:O	1:B:342:ASN:ND2	2.16	0.79
1:D:423:THR:HG21	1:D:460:LYS:HB3	1.68	0.76
1:A:219:ARG:NH1	1:A:486:VAL:O	2.20	0.74
1:A:182:GLU:OE2	1:A:219:ARG:NH2	2.25	0.70
1:A:371:GLN:O	1:A:375:MET:HG3	1.93	0.68
1:D:416:VAL:HG11	1:D:451:LEU:HD21	1.76	0.68
1:B:408:LYS:NZ	1:B:444:ASP:OD1	2.23	0.68
1:B:443:GLN:OE1	1:B:445:ARG:NH2	2.27	0.67
1:A:403:ASN:HA	1:A:406:LEU:HD23	1.77	0.66
1:B:242:GLY:O	2:B:501:HOH:O	2.14	0.66
1:C:416:VAL:HG11	1:C:451:LEU:HD11	1.77	0.66
1:A:364:PRO:HA	1:A:367:ILE:HD12	1.78	0.66
1:B:82:ALA:O	1:B:86:VAL:HG23	1.95	0.66
1:B:174:LEU:O	1:B:178:VAL:HG23	1.96	0.65
1:B:479:CYS:O	1:B:483:ILE:HD12	1.97	0.65
1:C:423:THR:HG21	1:C:461:LEU:HD21	1.78	0.64
1:D:126:VAL:HB	1:D:151:THR:HB	1.79	0.64
1:A:484:ASP:O	1:A:489:PRO:HD3	1.97	0.64
1:C:364:PRO:HA	1:C:367:ILE:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:ALA:HB1	1:C:261:MET:HG2	1.80	0.63
1:D:463:ARG:NH1	1:D:467:GLU:OE2	2.31	0.63
1:B:478:GLN:HB2	1:C:252:ILE:HD11	1.82	0.62
1:C:126:VAL:HB	1:C:151:THR:HB	1.81	0.61
1:A:175:ASP:O	2:A:501:HOH:O	2.16	0.61
1:D:420:LEU:HD11	1:D:424:LEU:HD12	1.81	0.61
1:A:448:LEU:HD11	1:A:466:LEU:HB3	1.83	0.61
1:D:130:VAL:O	1:D:134:VAL:HG23	2.01	0.61
1:B:412:VAL:HG11	1:B:472:PRO:HA	1.81	0.61
1:D:325:PRO:HG3	1:B:410:LEU:HD13	1.83	0.60
1:A:104:HIS:ND1	1:A:136:ASN:HB3	2.16	0.60
1:B:157:THR:HG21	1:B:235:LEU:HD12	1.83	0.60
1:C:204:PRO:HD3	1:C:411:ILE:HG12	1.84	0.59
1:D:431:ASP:O	1:D:435:GLU:HG2	2.02	0.59
1:A:148:GLY:HA3	1:A:247:LEU:HD21	1.84	0.59
1:B:167:LEU:HD22	1:B:225:LEU:HD21	1.85	0.58
1:C:77:LEU:HD22	1:C:105:CYS:HA	1.85	0.58
1:D:97:ALA:HA	1:D:141:LEU:HD23	1.86	0.58
1:D:139:ASP:HB2	1:D:141:LEU:HD13	1.85	0.58
1:B:364:PRO:HA	1:B:367:ILE:HD12	1.85	0.58
1:B:366:GLU:OE1	1:B:366:GLU:N	2.36	0.58
1:B:165:GLN:O	1:B:168:THR:OG1	2.21	0.57
1:D:329:ASN:O	1:D:331:ILE:N	2.37	0.57
1:A:120:GLU:HA	1:B:57:ILE:HD11	1.87	0.57
1:D:223:GLN:OE1	1:A:230:LYS:NZ	2.29	0.57
1:B:258:LEU:O	1:B:262:LEU:HD22	2.05	0.57
1:A:77:LEU:HD11	1:A:110:ILE:HD11	1.86	0.56
1:A:448:LEU:HD22	1:A:467:GLU:HG2	1.87	0.56
1:B:228:LEU:O	1:B:232:VAL:HG23	2.06	0.56
1:B:87:GLN:OE1	1:B:147:TRP:HB3	2.06	0.56
1:D:412:VAL:HG11	1:D:472:PRO:HA	1.88	0.56
1:B:206:THR:HG22	1:B:476:LEU:HD12	1.87	0.55
1:A:81:ALA:HB1	1:A:102:VAL:HG22	1.89	0.55
1:C:319:GLY:HA3	1:C:328:ASN:HA	1.88	0.55
1:A:126:VAL:HB	1:A:151:THR:HB	1.89	0.55
1:B:249:ASP:N	1:B:249:ASP:OD1	2.39	0.55
1:A:344:ARG:NH1	1:B:352:ASP:OD2	2.42	0.53
1:B:468:LYS:HD2	1:B:468:LYS:N	2.22	0.53
1:B:481:GLN:OE1	1:B:481:GLN:N	2.38	0.53
1:B:218:PHE:O	1:B:222:GLN:HG3	2.09	0.52
1:B:267:ALA:O	1:C:485:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:408:LYS:HB3	1:D:446:PRO:HA	1.91	0.51
1:A:448:LEU:CD1	1:A:466:LEU:HB3	2.40	0.51
1:C:412:VAL:HG11	1:C:472:PRO:HA	1.92	0.51
1:D:420:LEU:HD21	1:D:457:ILE:HG12	1.92	0.51
1:D:314:PHE:O	1:D:315:ILE:HD13	2.12	0.50
1:C:412:VAL:HG12	1:C:475:TYR:HD2	1.77	0.50
1:B:435:GLU:O	1:B:438:ARG:HB2	2.11	0.50
1:B:87:GLN:HA	1:B:92:ILE:HD13	1.92	0.50
1:D:445:ARG:NH2	1:D:449:ASP:HB3	2.26	0.50
1:C:168:THR:O	1:C:172:GLN:HG3	2.12	0.50
1:D:413:SER:O	1:D:417:MET:HG3	2.11	0.50
1:B:268:GLU:O	1:C:485:ARG:HD2	2.12	0.50
1:B:273:THR:HG22	1:B:356:SER:HB3	1.94	0.49
1:D:372:LEU:HB3	1:D:373:PRO:HD3	1.93	0.49
1:A:82:ALA:HB1	1:A:261:MET:HG2	1.94	0.49
1:A:416:VAL:HG11	1:A:451:LEU:HD11	1.95	0.49
1:B:138:LYS:O	1:B:141:LEU:HG	2.13	0.49
1:B:126:VAL:HB	1:B:151:THR:HB	1.96	0.48
1:A:104:HIS:CE1	1:A:136:ASN:HB3	2.48	0.48
1:D:407:SER:HB2	1:D:410:LEU:HB2	1.96	0.48
1:B:282:GLY:HA3	1:B:350:LEU:HD12	1.95	0.48
1:C:139:ASP:HB2	1:C:141:LEU:CD1	2.42	0.48
1:C:276:ASP:O	1:C:280:GLU:HG2	2.14	0.48
1:D:116:LYS:HE3	1:C:51:ALA:HB1	1.96	0.48
1:D:364:PRO:HA	1:D:367:ILE:HD12	1.96	0.48
1:B:231:ARG:HH12	1:C:227:GLU:CD	2.16	0.47
1:B:415:ALA:HB2	1:B:475:TYR:CD1	2.48	0.47
1:A:424:LEU:HD11	1:A:457:ILE:HG12	1.96	0.47
1:D:62:GLN:H	1:D:62:GLN:CD	2.15	0.47
1:B:163:ILE:HD11	1:B:372:LEU:HD21	1.96	0.47
1:C:97:ALA:HA	1:C:141:LEU:HD23	1.95	0.47
1:D:92:ILE:HD11	1:D:250:GLN:HB3	1.96	0.47
1:D:312:GLU:OE1	1:D:318:ARG:NH2	2.48	0.47
1:B:314:PHE:HD1	1:B:315:ILE:N	2.13	0.47
1:B:316:SER:OG	1:B:317:ASN:N	2.46	0.46
1:A:149:ALA:HB2	1:A:237:PHE:HE1	1.80	0.46
1:A:152:GLN:HA	1:A:155:THR:OG1	2.15	0.46
1:A:318:ARG:NH2	1:A:332:SER:OG	2.47	0.46
1:A:285:LEU:O	1:A:289:THR:OG1	2.26	0.46
1:A:273:THR:HG22	1:A:356:SER:HB3	1.98	0.46
1:C:408:LYS:HB3	1:C:446:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:LEU:HD12	1:D:420:LEU:O	2.15	0.46
1:B:404:LEU:HD22	1:B:472:PRO:HB2	1.96	0.46
1:A:120:GLU:HG2	1:B:57:ILE:HD11	1.97	0.45
1:C:139:ASP:HB2	1:C:141:LEU:HD13	1.98	0.45
1:B:56:ASP:OD1	1:B:64:ARG:NH2	2.43	0.45
1:C:461:LEU:HD12	1:C:465:GLU:HG2	1.97	0.45
1:D:426:ARG:NH2	1:A:144:TYR:HE1	2.14	0.45
1:D:463:ARG:O	1:D:467:GLU:HG2	2.16	0.45
1:A:87:GLN:OE1	1:A:147:TRP:HB3	2.16	0.45
1:A:116:LYS:O	1:A:120:GLU:HG3	2.17	0.45
1:C:127:LEU:O	1:C:131:GLN:HG3	2.16	0.45
1:D:318:ARG:HG2	1:D:331:ILE:HD11	1.99	0.44
1:A:414:GLU:OE1	1:A:475:TYR:OH	2.13	0.44
1:B:272:HIS:CG	1:B:360:ARG:HH21	2.35	0.44
1:C:282:GLY:HA3	1:C:350:LEU:HD12	2.00	0.44
1:D:271:TRP:HA	1:D:274:GLU:OE1	2.17	0.44
1:A:86:VAL:HG23	1:A:261:MET:HE2	1.99	0.44
1:B:92:ILE:HD12	1:B:92:ILE:H	1.82	0.44
1:C:463:ARG:O	1:C:467:GLU:HG3	2.17	0.44
1:A:94:PRO:HB2	1:A:96:ASN:OD1	2.17	0.44
1:A:100:GLU:HB3	1:A:141:LEU:HD23	2.00	0.44
1:D:414:GLU:O	1:D:418:MET:HG3	2.18	0.44
1:A:121:LEU:O	1:B:318:ARG:HA	2.18	0.43
1:B:127:LEU:O	1:B:131:GLN:HG3	2.18	0.43
1:B:213:ARG:HG3	1:C:269:ILE:HD13	1.98	0.43
1:A:163:ILE:HD11	1:A:372:LEU:HD21	1.99	0.43
1:B:325:PRO:O	1:B:327:LYS:N	2.52	0.43
1:B:94:PRO:HB2	1:B:96:ASN:OD1	2.18	0.43
1:C:227:GLU:O	1:C:230:LYS:HG2	2.19	0.43
1:A:167:LEU:HD13	1:A:225:LEU:HD11	2.00	0.43
1:A:404:LEU:HD22	1:A:472:PRO:HB2	2.00	0.43
1:B:420:LEU:HD21	1:B:457:ILE:HG12	2.00	0.43
1:B:480:SER:HA	1:B:483:ILE:HD12	1.99	0.43
1:C:235:LEU:HD21	1:C:258:LEU:HD23	1.99	0.43
1:C:247:LEU:HD12	1:C:251:GLY:HA2	2.00	0.43
1:A:131:GLN:O	1:A:134:VAL:HG22	2.18	0.43
1:A:173:ARG:HA	1:A:173:ARG:HD2	1.61	0.43
1:D:315:ILE:HB	1:D:318:ARG:HB2	2.01	0.43
1:D:385:ASN:O	1:D:389:VAL:HG23	2.19	0.43
1:C:188:HIS:O	1:C:191:VAL:HG12	2.19	0.42
1:A:318:ARG:HG2	1:A:331:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LYS:HD2	1:B:118:LYS:HA	1.88	0.42
1:C:87:GLN:OE1	1:C:147:TRP:HB3	2.20	0.42
1:C:183:HIS:NE2	1:C:187:GLN:OE1	2.53	0.42
1:B:420:LEU:CD1	1:B:461:LEU:HD12	2.49	0.42
1:B:411:ILE:HG23	1:B:412:VAL:HG13	2.01	0.42
1:D:51:ALA:HB1	1:C:116:LYS:HE3	2.01	0.41
1:B:271:TRP:HA	1:B:274:GLU:OE1	2.20	0.41
1:C:372:LEU:HD12	1:C:372:LEU:HA	1.91	0.41
1:B:314:PHE:C	1:B:314:PHE:CD1	2.94	0.41
1:B:148:GLY:HA3	1:B:247:LEU:HD21	2.01	0.41
1:D:417:MET:HG2	1:D:433:VAL:HB	2.01	0.41
1:A:304:GLN:HG2	1:C:199:LEU:HB3	2.02	0.41
1:B:258:LEU:O	1:B:261:MET:HB2	2.21	0.41
1:B:86:VAL:HG22	1:B:261:MET:HG3	2.02	0.41
1:B:485:ARG:HD2	1:C:268:GLU:O	2.20	0.41
1:C:469:LEU:HD23	1:C:469:LEU:HA	1.95	0.40
1:D:152:GLN:HG2	1:D:272:HIS:HD2	1.86	0.40
1:C:180:SER:OG	2:C:501:HOH:O	2.22	0.40
1:C:328:ASN:HA	1:C:328:ASN:HD22	1.67	0.40
1:C:462:ASP:OD1	1:C:462:ASP:N	2.54	0.40
1:D:352:ASP:OD2	1:C:344:ARG:NH1	2.54	0.40
1:A:318:ARG:O	1:A:320:SER:N	2.54	0.40
1:A:50:SER:C	1:A:52:GLY:H	2.25	0.40
1:A:460:LYS:O	1:A:461:LEU:HD23	2.21	0.40
1:B:156:ASP:O	1:B:160:VAL:HG23	2.21	0.40

All (2) 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:427:GLN:OE1	1:C:250:GLN:NE2[8_545]	2.10	0.10
1:A:427:GLN:NE2	1:C:90:LEU:O[8_545]	2.18	0.02

## 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	429/493 (87%)	410 (96%)	18 (4%)	1 (0%)	44	54
1	B	429/493 (87%)	412 (96%)	17 (4%)	0	100	100
1	C	433/493 (88%)	414 (96%)	18 (4%)	1 (0%)	44	54
1	D	431/493 (87%)	414 (96%)	16 (4%)	1 (0%)	44	54
All	All	1722/1972 (87%)	1650 (96%)	69 (4%)	3 (0%)	44	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	326	GLN
1	D	329	ASN
1	A	142	GLY

### 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	355/404 (88%)	350 (99%)	5 (1%)	62	77
1	B	356/404 (88%)	350 (98%)	6 (2%)	56	71
1	C	356/404 (88%)	353 (99%)	3 (1%)	79	88
1	D	358/404 (89%)	356 (99%)	2 (1%)	84	92
All	All	1425/1616 (88%)	1409 (99%)	16 (1%)	70	83

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	321	SER
1	D	488	SER
1	A	143	GLU
1	A	173	ARG
1	A	230	LYS

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Mol	Chain	Res	Type
1	A	463	ARG
1	A	467	GLU
1	B	231	ARG
1	B	262	LEU
1	B	314	PHE
1	B	315	ILE
1	B	426	ARG
1	B	485	ARG
1	C	268	GLU
1	C	423	THR
1	C	463	ARG

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

Mol	Chain	Res	Type
1	D	190	ASN
1	B	104	HIS
1	B	478	GLN
1	C	328	ASN
1	C	430	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 [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	320:SER	C	323:THR	N	6.43

## 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	436/493 (88%)	0.51	24 (5%) 32 34	51, 68, 94, 138	0
1	B	434/493 (88%)	1.03	59 (13%) 8 9	55, 81, 109, 122	0
1	C	439/493 (89%)	0.53	21 (4%) 36 39	53, 72, 98, 127	0
1	D	437/493 (88%)	0.38	15 (3%) 48 51	50, 68, 102, 126	0
All	All	1746/1972 (88%)	0.61	119 (6%) 25 27	50, 72, 104, 138	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	324	MET	7.9
1	B	325	PRO	7.6
1	C	324	MET	7.2
1	B	457	ILE	6.2
1	A	320	SER	6.1
1	B	319	GLY	6.1
1	A	325	PRO	5.9
1	A	324	MET	4.7
1	B	489	PRO	4.7
1	D	325	PRO	4.5
1	C	45	PRO	4.4
1	A	462	ASP	4.3
1	D	327	LYS	4.3
1	A	90	LEU	4.2
1	A	144	TYR	4.2
1	A	328	ASN	4.1
1	C	489	PRO	4.1
1	A	326	GLN	4.1
1	A	489	PRO	4.0
1	D	321	SER	4.0
1	C	47	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	327	LYS	3.9
1	C	320	SER	3.8
1	B	51	ALA	3.7
1	B	105	CYS	3.7
1	B	327	LYS	3.7
1	B	84	ALA	3.6
1	A	248	GLY	3.6
1	C	46	ASP	3.6
1	C	251	GLY	3.6
1	B	98	ALA	3.6
1	D	320	SER	3.3
1	B	102	VAL	3.3
1	D	50	SER	3.3
1	A	143	GLU	3.3
1	C	319	GLY	3.2
1	B	151	THR	3.1
1	B	81	ALA	3.1
1	C	252	ILE	3.0
1	B	240	ALA	3.0
1	B	85	ILE	3.0
1	B	141	LEU	3.0
1	A	323	THR	2.9
1	C	50	SER	2.9
1	B	93	ILE	2.9
1	A	70	GLN	2.9
1	B	134	VAL	2.9
1	C	141	LEU	2.9
1	D	455	HIS	2.9
1	B	140	GLY	2.9
1	B	101	ILE	2.9
1	C	461	LEU	2.9
1	B	315	ILE	2.8
1	D	442	VAL	2.8
1	D	489	PRO	2.8
1	A	149	ALA	2.8
1	A	86	VAL	2.8
1	A	315	ILE	2.8
1	B	441	PHE	2.8
1	B	97	ALA	2.7
1	A	112	TRP	2.7
1	B	135	ALA	2.7
1	C	142	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	145	CYS	2.7
1	B	451	LEU	2.7
1	A	441	PHE	2.7
1	B	144	TYR	2.7
1	B	458	ALA	2.7
1	C	90	LEU	2.6
1	A	51	ALA	2.6
1	B	107	VAL	2.5
1	C	151	THR	2.5
1	D	434	TYR	2.5
1	B	79	ILE	2.5
1	A	50	SER	2.5
1	A	314	PHE	2.5
1	B	139	ASP	2.4
1	B	77	LEU	2.4
1	B	90	LEU	2.4
1	B	133	LEU	2.4
1	B	262	LEU	2.4
1	B	412	VAL	2.4
1	D	151	THR	2.4
1	B	261	MET	2.4
1	B	138	LYS	2.4
1	B	410	LEU	2.4
1	B	83	LEU	2.4
1	B	253	ALA	2.4
1	B	467	GLU	2.3
1	B	50	SER	2.3
1	B	418	MET	2.3
1	B	434	TYR	2.3
1	B	476	LEU	2.3
1	B	94	PRO	2.3
1	D	457	ILE	2.3
1	B	126	VAL	2.3
1	B	147	TRP	2.3
1	C	269	ILE	2.3
1	D	328	ASN	2.2
1	B	86	VAL	2.2
1	B	142	GLY	2.2
1	C	317	ASN	2.2
1	C	424	LEU	2.2
1	A	318	ARG	2.2
1	B	99	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	51	ALA	2.2
1	B	209	PHE	2.2
1	B	118	LYS	2.2
1	B	54	LEU	2.2
1	C	452	LEU	2.1
1	B	88	ALA	2.1
1	C	129	ILE	2.1
1	A	247	LEU	2.1
1	B	112	TRP	2.1
1	B	121	LEU	2.1
1	B	205	ILE	2.1
1	B	67	TRP	2.1
1	A	147	TRP	2.0
1	D	57	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.