



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:39 PM GMT

PDB ID : 1ULT  
Title : Crystal structure of tt0168 from *Thermus thermophilus* HB8  
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Deposited on : 2003-09-16  
Resolution : 2.55 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

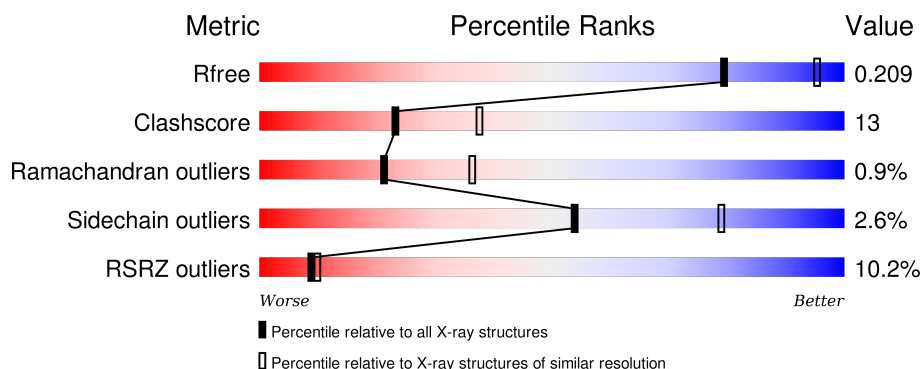
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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))
$R_{free}$	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	541	<div> <div>5%</div> <div>72%</div> <div>26%</div> <div>..</div> </div>
1	B	541	<div> <div>15%</div> <div>72%</div> <div>22%</div> <div>• 5%</div> </div>

## 2 Entry composition [i](#)

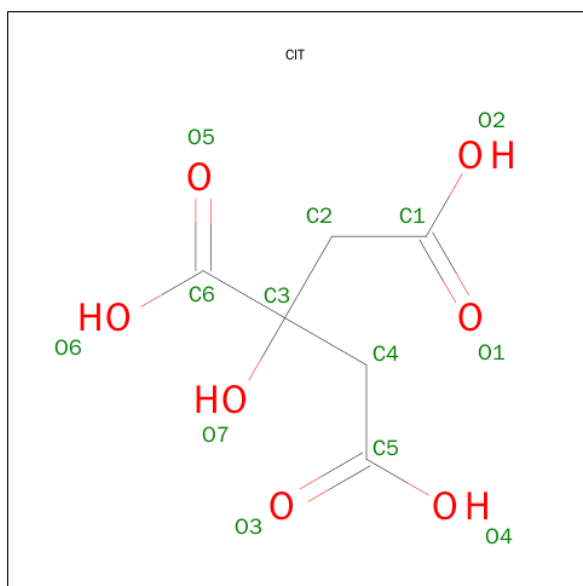
There are 3 unique types of molecules in this entry. The entry contains 8431 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 long chain fatty acid-CoA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	0	0
			4142	2653	721	757	11			
1	B	514	Total	C	N	O	S	0	0	0
			3989	2551	693	734	11			

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	153	Total	O	0	0
			153	153		

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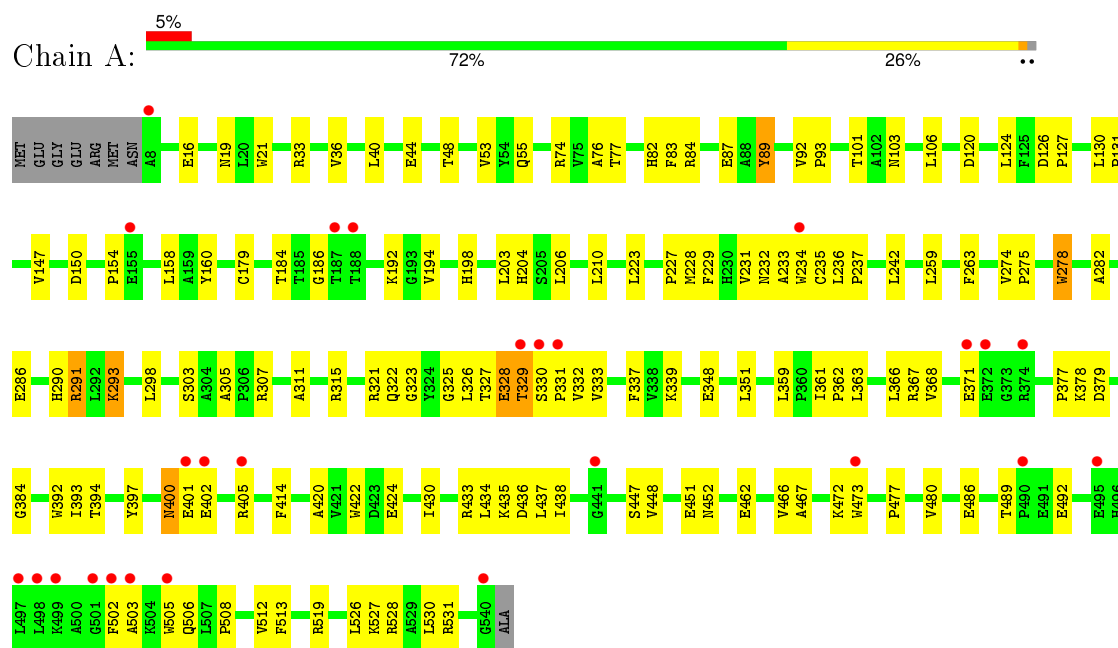
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	134	Total 134	O 134	0	0

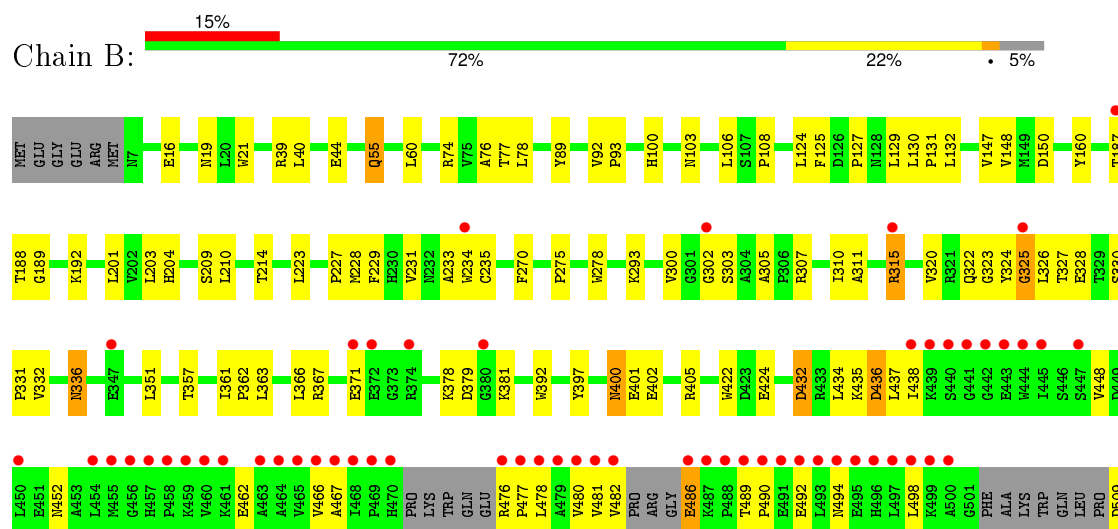
### 3 Residue-property plots [i](#)

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.

- Molecule 1: long chain fatty acid-CoA ligase



- Molecule 1: long chain fatty acid-CoA ligase



A510	T511	V512	F513	A514	E515	E516	T517	P518	R519	T520	SER	ALA	GLY	LYS	F525	L526	K527	R528	A529	L530	R531	E532	Q533	Y534	K535	N536	Y537	Y538	G539	GLY	ALA

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.95Å 124.69Å 212.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.64 – 2.55 49.64 – 2.54	Depositor EDS
% Data completeness (in resolution range)	97.4 (49.64-2.55) 97.0 (49.64-2.54)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.51 (at 2.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.206 , 0.239 0.208 , 0.209	Depositor DCC
$R_{free}$ test set	2442 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.6	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 48301 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8431	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CIT

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	0.34	0/4242	0.59	0/5765
1	B	0.34	0/4077	0.58	0/5535
All	All	0.34	0/8319	0.58	0/11300

There are no bond length outliers.

There are no bond angle outliers.

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	4142	0	4165	122	0
1	B	3989	0	4008	101	0
2	A	13	0	5	3	0
3	A	153	0	0	5	0
3	B	134	0	0	1	0
All	All	8431	0	8178	219	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 (219) 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:329:THR:CG2	1:A:394:THR:HG22	1.89	1.02
1:A:329:THR:HG22	1:A:394:THR:HG22	1.42	0.97
1:A:330:SER:HB3	1:A:393:ILE:HD13	1.61	0.82
1:B:92:VAL:HB	1:B:93:PRO:HD3	1.67	0.77
1:B:315:ARG:HH11	1:B:315:ARG:HG3	1.50	0.76
1:B:325:GLY:HA2	1:B:330:SER:O	1.85	0.76
1:A:311:ALA:HB1	1:A:315:ARG:HH12	1.53	0.73
1:A:329:THR:HG23	1:A:394:THR:HG22	1.69	0.73
1:A:92:VAL:HB	1:A:93:PRO:HD3	1.72	0.71
1:B:231:VAL:HG21	1:B:326:LEU:HA	1.73	0.70
1:B:438:ILE:HD13	1:B:477:PRO:HB3	1.75	0.69
1:A:435:LYS:NZ	2:A:1001:CIT:H42	2.09	0.67
1:A:329:THR:HG22	1:A:394:THR:CG2	2.24	0.66
1:A:433:ARG:HG3	1:A:434:LEU:HD13	1.76	0.66
1:B:432:ASP:HA	1:B:448:VAL:HG21	1.76	0.66
1:A:477:PRO:HG2	1:A:508:PRO:HA	1.78	0.66
1:B:401:GLU:O	1:B:405:ARG:HG3	1.95	0.65
1:A:307:ARG:NH1	1:A:351:LEU:HD23	2.11	0.65
1:A:210:LEU:HD23	1:B:210:LEU:HD23	1.77	0.65
1:B:432:ASP:OD1	1:B:448:VAL:HG23	1.97	0.65
1:B:275:PRO:HG2	1:B:303:SER:HB2	1.79	0.65
1:B:489:THR:OG1	1:B:492:GLU:HG3	1.98	0.64
1:A:194:VAL:HG21	1:A:328:GLU:HA	1.80	0.64
1:A:435:LYS:HD3	2:A:1001:CIT:H22	1.78	0.64
1:A:402:GLU:HG2	1:A:405:ARG:NH2	2.14	0.62
1:B:307:ARG:NH1	1:B:351:LEU:HD23	2.13	0.62
1:B:325:GLY:HA3	1:B:331:PRO:O	1.98	0.62
1:A:435:LYS:HZ1	2:A:1001:CIT:H42	1.65	0.62
1:A:329:THR:HG21	1:A:414:PHE:CD2	2.34	0.62
1:A:234:TRP:HH2	1:A:323:GLY:HA3	1.64	0.62
1:A:311:ALA:HB1	1:A:315:ARG:NH1	2.15	0.61
1:A:438:ILE:HD13	1:A:477:PRO:HB3	1.83	0.61
1:A:231:VAL:CG1	1:A:327:THR:HA	2.30	0.61
1:B:536:ASN:OD1	1:B:539:GLY:HA2	2.00	0.60
1:A:489:THR:OG1	1:A:492:GLU:HG3	2.02	0.60
1:B:327:THR:HG23	1:B:330:SER:H	1.65	0.60
1:A:400:ASN:HD22	1:A:400:ASN:C	2.03	0.60
1:B:476:ARG:CZ	1:B:476:ARG:HA	2.31	0.60
1:B:231:VAL:HG12	1:B:231:VAL:O	2.01	0.60
1:A:275:PRO:HG2	1:A:303:SER:HB2	1.83	0.59
1:A:401:GLU:O	1:A:405:ARG:HG3	2.02	0.59
1:A:326:LEU:N	1:A:326:LEU:HD12	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ARG:HG3	1:A:434:LEU:CD1	2.32	0.58
1:A:84:ARG:HD3	1:A:160:TYR:CD1	2.38	0.58
1:B:400:ASN:C	1:B:400:ASN:HD22	2.06	0.58
1:B:512:VAL:HG12	1:B:513:PHE:N	2.19	0.57
1:A:329:THR:HG22	1:A:394:THR:N	2.19	0.57
1:A:420:ALA:HB2	1:A:430:ILE:HA	1.87	0.57
1:A:433:ARG:HA	1:A:437:LEU:HD12	1.87	0.57
1:A:311:ALA:O	1:A:315:ARG:HG3	2.05	0.56
1:A:329:THR:HG21	1:A:414:PHE:CG	2.41	0.56
1:A:325:GLY:HA3	1:A:331:PRO:O	2.06	0.55
1:B:315:ARG:NH1	1:B:315:ARG:HG3	2.21	0.55
1:B:366:LEU:HD23	1:B:367:ARG:N	2.21	0.55
1:A:203:LEU:HD21	1:B:203:LEU:HD21	1.87	0.54
1:A:321:ARG:HD3	3:A:1064:HOH:O	2.08	0.54
1:A:83:PHE:CZ	1:A:84:ARG:NH1	2.75	0.54
1:B:234:TRP:HH2	1:B:323:GLY:HA3	1.73	0.54
1:B:201:LEU:HD13	3:B:615:HOH:O	2.08	0.54
1:B:39:ARG:HH11	1:B:39:ARG:HG3	1.73	0.53
1:A:19:ASN:HD22	1:A:21:TRP:H	1.55	0.53
1:B:462:GLU:CD	1:B:519:ARG:HH22	2.12	0.53
1:A:103:ASN:HB3	1:A:106:LEU:HG	1.90	0.53
1:B:233:ALA:O	1:B:234:TRP:HB2	2.07	0.53
1:A:305:ALA:H	1:A:322:GLN:HE21	1.57	0.53
1:A:223:LEU:C	1:A:223:LEU:HD23	2.29	0.53
1:A:526:LEU:CD2	1:A:528:ARG:HB3	2.38	0.53
1:A:466:VAL:HG12	1:A:527:LYS:HD3	1.90	0.53
1:A:512:VAL:HG12	1:A:513:PHE:N	2.24	0.52
1:A:234:TRP:CH2	1:A:323:GLY:HA3	2.41	0.52
1:B:223:LEU:C	1:B:223:LEU:HD23	2.30	0.52
1:B:527:LYS:O	1:B:531:ARG:HG3	2.10	0.52
1:A:40:LEU:HD12	1:A:44:GLU:CG	2.39	0.52
1:B:204:HIS:NE2	1:B:332:VAL:HB	2.24	0.52
1:B:476:ARG:HA	1:B:476:ARG:NE	2.25	0.52
1:B:366:LEU:C	1:B:366:LEU:HD23	2.31	0.51
1:A:526:LEU:HD23	1:A:528:ARG:HB3	1.92	0.51
1:A:74:ARG:HD3	1:A:74:ARG:N	2.25	0.51
1:B:432:ASP:HA	1:B:448:VAL:CG2	2.39	0.51
1:A:124:LEU:HD23	1:A:147:VAL:HB	1.93	0.51
1:B:378:LYS:HB2	1:B:424:GLU:OE2	2.09	0.51
1:A:278:TRP:HA	1:A:278:TRP:CE3	2.45	0.51
1:B:526:LEU:HD23	1:B:528:ARG:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:THR:HA	1:A:394:THR:HB	1.92	0.51
1:A:502:PHE:HA	1:A:506:GLN:NE2	2.26	0.51
1:B:311:ALA:O	1:B:315:ARG:HG3	2.10	0.50
1:A:329:THR:HG22	1:A:394:THR:H	1.75	0.50
1:A:19:ASN:ND2	1:A:21:TRP:H	2.08	0.50
1:A:480:VAL:HG21	1:A:530:LEU:HD22	1.93	0.50
1:A:330:SER:CB	1:A:333:VAL:HG13	2.41	0.50
1:B:209:SER:HA	1:B:214:THR:OG1	2.11	0.50
1:A:278:TRP:HA	1:A:278:TRP:HE3	1.75	0.50
1:B:438:ILE:HG12	1:B:467:ALA:HB2	1.94	0.50
1:B:234:TRP:O	1:B:235:CYS:HB2	2.12	0.50
1:B:278:TRP:HA	1:B:278:TRP:CE3	2.47	0.50
1:B:509:ASP:O	1:B:510:ALA:HB2	2.12	0.50
1:A:361:ILE:HD11	1:A:392:TRP:CZ2	2.46	0.50
1:B:60:LEU:HD22	1:B:160:TYR:OH	2.11	0.49
1:B:103:ASN:HB3	1:B:106:LEU:HG	1.94	0.49
1:A:531:ARG:HD2	3:A:1134:HOH:O	2.11	0.49
1:B:187:THR:O	1:B:189:GLY:N	2.46	0.49
1:A:76:ALA:HB2	1:A:120:ASP:OD2	2.13	0.49
1:A:433:ARG:HA	1:A:437:LEU:HB2	1.95	0.49
1:A:101:THR:HB	1:A:229:PHE:HA	1.95	0.49
1:A:330:SER:HB2	1:A:333:VAL:HG13	1.94	0.48
1:A:462:GLU:CD	1:A:519:ARG:HH22	2.15	0.48
1:B:325:GLY:CA	1:B:330:SER:O	2.56	0.48
1:B:526:LEU:CD2	1:B:528:ARG:HB3	2.43	0.48
1:B:436:ASP:HA	1:B:531:ARG:HH21	1.78	0.48
1:A:130:LEU:HB3	1:A:131:PRO:HD3	1.96	0.48
1:B:402:GLU:HG2	1:B:405:ARG:NH2	2.29	0.48
1:B:234:TRP:CH2	1:B:323:GLY:HA3	2.49	0.48
1:A:33:ARG:HD2	3:A:1078:HOH:O	2.14	0.47
1:A:527:LYS:O	1:A:531:ARG:HG3	2.14	0.47
1:A:124:LEU:CD2	1:A:147:VAL:HB	2.45	0.47
1:B:278:TRP:HA	1:B:278:TRP:HE3	1.78	0.47
1:A:377:PRO:HB2	1:A:379:ASP:OD2	2.14	0.47
1:B:124:LEU:CD2	1:B:147:VAL:HB	2.44	0.47
1:A:378:LYS:HB2	1:A:424:GLU:OE2	2.14	0.47
1:B:74:ARG:N	1:B:74:ARG:HD3	2.30	0.47
1:B:466:VAL:HG12	1:B:527:LYS:HD3	1.97	0.47
1:A:361:ILE:HD11	1:A:392:TRP:HZ2	1.80	0.47
1:B:227:PRO:HB3	1:B:229:PHE:CE2	2.50	0.47
1:B:40:LEU:HD12	1:B:44:GLU:CG	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:ALA:CB	1:B:315:ARG:HH12	2.28	0.46
1:B:305:ALA:H	1:B:322:GLN:HE21	1.62	0.46
1:A:82:HIS:HE1	1:A:126:ASP:OD1	1.98	0.46
1:B:39:ARG:NH1	1:B:39:ARG:HG3	2.30	0.46
1:A:228:MET:HA	1:A:233:ALA:HB2	1.97	0.46
1:A:366:LEU:HD23	1:A:366:LEU:C	2.35	0.46
1:A:438:ILE:CD1	1:A:477:PRO:HB3	2.45	0.46
1:B:478:LEU:HD11	1:B:512:VAL:HG23	1.96	0.46
1:A:366:LEU:HD23	1:A:367:ARG:N	2.31	0.46
1:A:242:LEU:HD11	1:B:362:PRO:HB3	1.97	0.46
1:A:274:VAL:HG22	3:A:1093:HOH:O	2.15	0.46
1:A:290:HIS:O	1:A:291:ARG:HD3	2.16	0.46
1:A:77:THR:HA	1:A:124:LEU:O	2.16	0.45
1:A:89:TYR:OH	1:A:232:ASN:HA	2.16	0.45
1:B:19:ASN:ND2	1:B:21:TRP:H	2.15	0.45
1:B:192:LYS:HB3	1:B:397:TYR:CD1	2.50	0.45
1:A:53:VAL:HG13	1:A:87:GLU:HG2	1.98	0.45
1:B:336:ASN:HD22	1:B:336:ASN:C	2.20	0.45
1:B:494:ASN:O	1:B:498:LEU:HG	2.17	0.45
1:B:311:ALA:C	1:B:315:ARG:NH1	2.69	0.45
1:A:447:SER:O	1:A:451:GLU:HG2	2.16	0.45
1:B:311:ALA:HB1	1:B:315:ARG:HH12	1.82	0.45
1:B:481:VAL:HG12	1:B:482:VAL:N	2.32	0.45
1:B:438:ILE:CD1	1:B:477:PRO:HB3	2.46	0.45
1:A:179:CYS:HB3	1:A:198:HIS:CD2	2.52	0.44
1:B:108:PRO:HG3	1:B:132:LEU:CD1	2.47	0.44
1:B:324:TYR:HB2	1:B:357:THR:CG2	2.48	0.44
1:A:127:PRO:HG3	1:A:150:ASP:HB2	1.99	0.44
1:A:330:SER:HB3	1:A:393:ILE:CD1	2.41	0.44
1:A:282:ALA:O	1:A:286:GLU:HG3	2.17	0.44
1:A:330:SER:CB	1:A:333:VAL:CG1	2.96	0.44
1:A:503:ALA:HB3	1:A:505:TRP:CD1	2.53	0.44
1:B:512:VAL:CG1	1:B:513:PHE:N	2.81	0.44
1:A:274:VAL:HG13	3:A:1093:HOH:O	2.18	0.43
1:A:147:VAL:HA	1:A:158:LEU:O	2.18	0.43
1:B:127:PRO:HG3	1:B:150:ASP:HB2	2.00	0.43
1:A:305:ALA:H	1:A:322:GLN:NE2	2.16	0.43
1:B:55:GLN:HB3	1:B:55:GLN:HE21	1.68	0.43
1:B:361:ILE:HD11	1:B:392:TRP:CZ2	2.54	0.43
1:B:361:ILE:HD11	1:B:392:TRP:HZ2	1.84	0.43
1:A:130:LEU:HD21	1:A:154:PRO:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:PHE:CZ	1:B:148:VAL:HG22	2.53	0.43
1:B:379:ASP:OD1	1:B:381:LYS:N	2.45	0.43
1:A:184:THR:HG21	1:A:328:GLU:OE2	2.18	0.43
1:B:76:ALA:HA	1:B:100:HIS:O	2.19	0.43
1:B:448:VAL:HG12	1:B:452:ASN:ND2	2.33	0.43
1:B:400:ASN:C	1:B:400:ASN:ND2	2.71	0.43
1:A:400:ASN:ND2	1:A:400:ASN:C	2.71	0.43
1:A:448:VAL:HG12	1:A:452:ASN:ND2	2.34	0.43
1:B:302:GLY:HA3	1:B:326:LEU:HD23	2.01	0.42
1:B:490:PRO:O	1:B:494:ASN:ND2	2.53	0.42
1:B:310:ILE:HG23	1:B:320:VAL:HB	2.00	0.42
1:B:19:ASN:ND2	1:B:21:TRP:HB3	2.34	0.42
1:B:476:ARG:HG2	1:B:476:ARG:HH11	1.84	0.42
1:A:307:ARG:NH2	1:A:348:GLU:O	2.52	0.42
1:B:77:THR:HA	1:B:124:LEU:O	2.19	0.42
1:A:298:LEU:HD23	1:A:298:LEU:C	2.39	0.42
1:A:36:VAL:HB	1:A:48:THR:HG23	2.02	0.42
1:A:83:PHE:O	1:A:87:GLU:HG3	2.19	0.42
1:B:228:MET:HA	1:B:233:ALA:HB2	2.02	0.42
1:B:270:PHE:C	1:B:270:PHE:CD1	2.93	0.42
1:A:486:GLU:O	1:A:486:GLU:HG3	2.18	0.42
1:A:503:ALA:O	1:A:506:GLN:HG2	2.19	0.42
1:B:476:ARG:NH2	1:B:477:PRO:HD2	2.33	0.42
1:B:204:HIS:HD2	1:B:392:TRP:CE2	2.38	0.42
1:A:293:LYS:HD2	1:A:293:LYS:H	1.84	0.42
1:A:436:ASP:OD1	1:A:448:VAL:HG23	2.20	0.42
1:B:124:LEU:HD23	1:B:147:VAL:HB	2.01	0.41
1:A:502:PHE:HA	1:A:506:GLN:HE21	1.84	0.41
1:A:259:LEU:HB3	1:A:263:PHE:CE2	2.55	0.41
1:A:368:VAL:HG12	1:A:384:GLY:HA3	2.02	0.41
1:A:512:VAL:CG1	1:A:513:PHE:N	2.83	0.41
1:B:325:GLY:HA3	1:B:331:PRO:C	2.40	0.41
1:A:234:TRP:O	1:A:235:CYS:HB2	2.20	0.41
1:B:78:LEU:O	1:B:129:LEU:HD12	2.20	0.41
1:A:337:PHE:CE1	1:A:359:LEU:HD12	2.56	0.41
1:B:435:LYS:C	1:B:437:LEU:H	2.23	0.41
1:A:329:THR:CB	1:A:394:THR:H	2.33	0.41
1:A:326:LEU:C	1:A:328:GLU:N	2.74	0.41
1:B:519:ARG:HB3	1:B:520:THR:H	1.69	0.41
1:B:486:GLU:N	1:B:486:GLU:OE1	2.53	0.41
1:B:130:LEU:N	1:B:131:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LYS:HB3	1:A:397:TYR:CD1	2.56	0.40
1:A:236:LEU:HB2	1:A:237:PRO:HD3	2.02	0.40
1:A:438:ILE:HG12	1:A:467:ALA:HB2	2.04	0.40
1:A:227:PRO:HB3	1:A:229:PHE:CE2	2.57	0.40
1:B:300:VAL:HG21	1:B:305:ALA:HB2	2.03	0.40
1:A:330:SER:HA	1:A:331:PRO:HD3	1.94	0.40
1:B:480:VAL:HG21	1:B:530:LEU:HD22	2.03	0.40
1:A:362:PRO:O	1:A:363:LEU:HB2	2.20	0.40
1:A:206:LEU:HD11	1:B:363:LEU:HD11	2.03	0.40
1:A:84:ARG:HH21	1:A:150:ASP:HA	1.86	0.40
1:A:76:ALA:HB2	1:A:120:ASP:CG	2.42	0.40
1:B:328:GLU:H	1:B:328:GLU:CD	2.25	0.40
1:A:204:HIS:NE2	1:A:332:VAL:HB	2.37	0.40

There are no symmetry-related clashes.

## 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	531/541 (98%)	510 (96%)	17 (3%)	4 (1%)	24	40
1	B	504/541 (93%)	484 (96%)	15 (3%)	5 (1%)	19	33
All	All	1035/1082 (96%)	994 (96%)	32 (3%)	9 (1%)	21	36

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	188	THR
1	B	434	LEU
1	A	328	GLU
1	A	329	THR
1	B	432	ASP

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Mol	Chain	Res	Type
1	A	472	LYS
1	B	510	ALA
1	A	186	GLY
1	B	325	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	431/437 (99%)	420 (97%)	11 (3%)	54	79
1	B	417/437 (95%)	406 (97%)	11 (3%)	54	79
All	All	848/874 (97%)	826 (97%)	22 (3%)	54	79

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	55	GLN
1	A	89	TYR
1	A	278	TRP
1	A	291	ARG
1	A	293	LYS
1	A	339	LYS
1	A	371	GLU
1	A	400	ASN
1	A	422	TRP
1	A	473	TRP
1	B	16	GLU
1	B	55	GLN
1	B	89	TYR
1	B	293	LYS
1	B	315	ARG
1	B	336	ASN
1	B	371	GLU
1	B	400	ASN

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Mol	Chain	Res	Type
1	B	422	TRP
1	B	436	ASP
1	B	486	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	55	GLN
1	A	82	HIS
1	A	128	ASN
1	A	144	GLN
1	A	290	HIS
1	A	322	GLN
1	A	335	GLN
1	A	400	ASN
1	A	452	ASN
1	A	474	GLN
1	A	506	GLN
1	B	19	ASN
1	B	55	GLN
1	B	128	ASN
1	B	144	GLN
1	B	290	HIS
1	B	322	GLN
1	B	335	GLN
1	B	336	ASN
1	B	400	ASN
1	B	452	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 carbohydrates in this entry.

## 5.6 Ligand geometry

1 ligand is 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	CIT	A	1001	-	3,12,12	2.57	1 (33%)	3,17,17	3.15	2 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	A	1001	-	-	0/6/16/16	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	CIT	O7-C3	4.17	1.49	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	CIT	C3-C4-C5	3.20	120.08	114.96
2	A	1001	CIT	C3-C2-C1	4.39	121.98	114.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	CIT	3	0

## 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

### 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	533/541 (98%)	0.18	26 (4%) 33 39	16, 36, 71, 81	0
1	B	514/541 (95%)	0.60	81 (15%) 3 3	17, 34, 112, 123	0
All	All	1047/1082 (96%)	0.39	107 (10%) 9 10	16, 35, 107, 123	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	511	TYR	9.0
1	B	500	ALA	8.3
1	B	468	ILE	7.9
1	B	478	LEU	7.8
1	B	490	PRO	7.5
1	A	329	THR	7.4
1	B	493	LEU	7.2
1	B	497	LEU	6.8
1	B	441	GLY	6.7
1	B	463	ALA	6.6
1	B	458	PRO	6.1
1	B	538	TYR	6.1
1	B	526	LEU	6.0
1	B	489	THR	6.0
1	B	536	ASN	5.9
1	B	440	SER	5.9
1	B	510	ALA	5.6
1	B	444	TRP	5.5
1	B	537	TYR	5.3
1	B	439	LYS	5.2
1	B	496	HIS	5.0
1	B	488	PRO	4.8
1	B	528	ARG	4.8
1	A	405	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	495	GLU	4.8
1	B	477	PRO	4.6
1	A	495	GLU	4.6
1	B	371	GLU	4.5
1	B	534	TYR	4.3
1	B	494	ASN	4.2
1	B	532	GLU	4.2
1	B	516	GLU	4.1
1	B	459	LYS	4.1
1	B	530	LEU	4.1
1	B	491	GLU	4.0
1	B	481	VAL	3.9
1	B	513	PHE	3.9
1	B	325	GLY	3.9
1	B	492	GLU	3.9
1	B	438	ILE	3.9
1	B	464	ALA	3.9
1	B	467	ALA	3.8
1	B	443	GLU	3.8
1	B	470	HIS	3.8
1	B	486	GLU	3.7
1	B	457	HIS	3.7
1	B	469	PRO	3.6
1	B	529	ALA	3.6
1	B	445	ILE	3.5
1	B	466	VAL	3.5
1	B	482	VAL	3.5
1	B	499	LYS	3.5
1	A	234	TRP	3.4
1	A	372	GLU	3.3
1	A	502	PHE	3.3
1	A	8	ALA	3.3
1	A	330	SER	3.3
1	A	401	GLU	3.2
1	A	501	GLY	3.2
1	B	455	MET	3.2
1	B	187	THR	3.1
1	B	460	VAL	3.1
1	A	505	TRP	3.1
1	B	442	GLY	3.1
1	A	371	GLU	3.0
1	B	456	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	498	LEU	2.9
1	B	539	GLY	2.9
1	B	487	LYS	2.9
1	B	302	GLY	2.8
1	B	374	ARG	2.8
1	B	476	ARG	2.8
1	B	372	GLU	2.8
1	B	515	GLU	2.8
1	A	497	LEU	2.7
1	B	533	GLN	2.7
1	B	447	SER	2.7
1	B	315	ARG	2.7
1	A	441	GLY	2.7
1	B	520	THR	2.6
1	A	503	ALA	2.6
1	B	517	ILE	2.6
1	A	188	THR	2.5
1	B	234	TRP	2.5
1	B	512	VAL	2.5
1	B	450	LEU	2.5
1	A	331	PRO	2.5
1	B	465	VAL	2.4
1	B	480	VAL	2.4
1	A	402	GLU	2.4
1	A	498	LEU	2.4
1	A	499	LYS	2.4
1	B	527	LYS	2.4
1	A	155	GLU	2.3
1	B	380	GLY	2.3
1	B	461	LYS	2.3
1	A	187	THR	2.3
1	A	473	TRP	2.3
1	B	454	LEU	2.2
1	B	479	ALA	2.2
1	A	540	GLY	2.2
1	B	535	LYS	2.2
1	B	347	GLU	2.2
1	B	514	ALA	2.2
1	A	374	ARG	2.1
1	B	525	PHE	2.0
1	A	490	PRO	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CIT	A	1001	13/13	0.81	0.21	0.46	81,84,87,87	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.