Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:27 pm BST

PDB ID	:	1ULT
Title	:	Crystal structure of tt0168 from Thermus thermophilus HB8
Authors	:	Hisanaga, Y.; Ago, H.; Nakatsu, T.; Hamada, K.; Ida, K.; Kanda, H.; Yamamoto, M.; Hori, T.; Arii, Y.; Sugahara, M.; Kuramitsu, S.; Yokoyama, S.; Miyano, M.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/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:

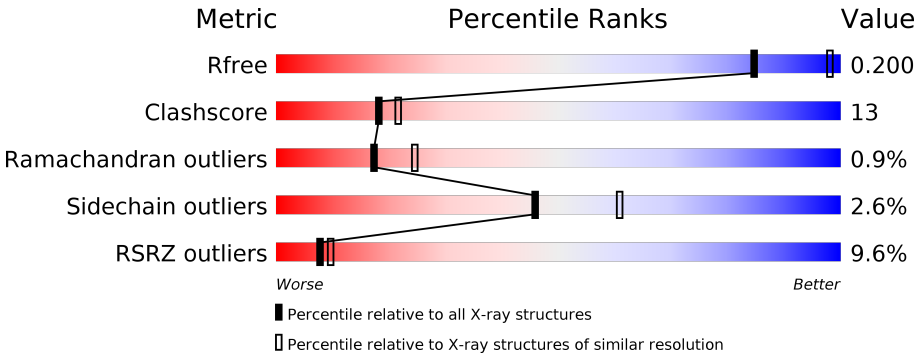
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 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 <=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	5% 72% 26% ··
1	B	541	14% 72% 22% · 5%

2 Entry composition

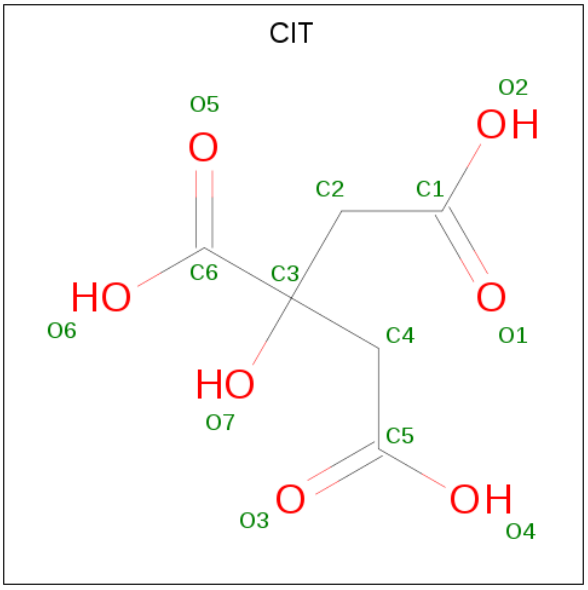
There are 3 unique types of molecules in this entry. The entry contains 8431 atoms, of which 0 are hydrogens and 0 are deuteriums.

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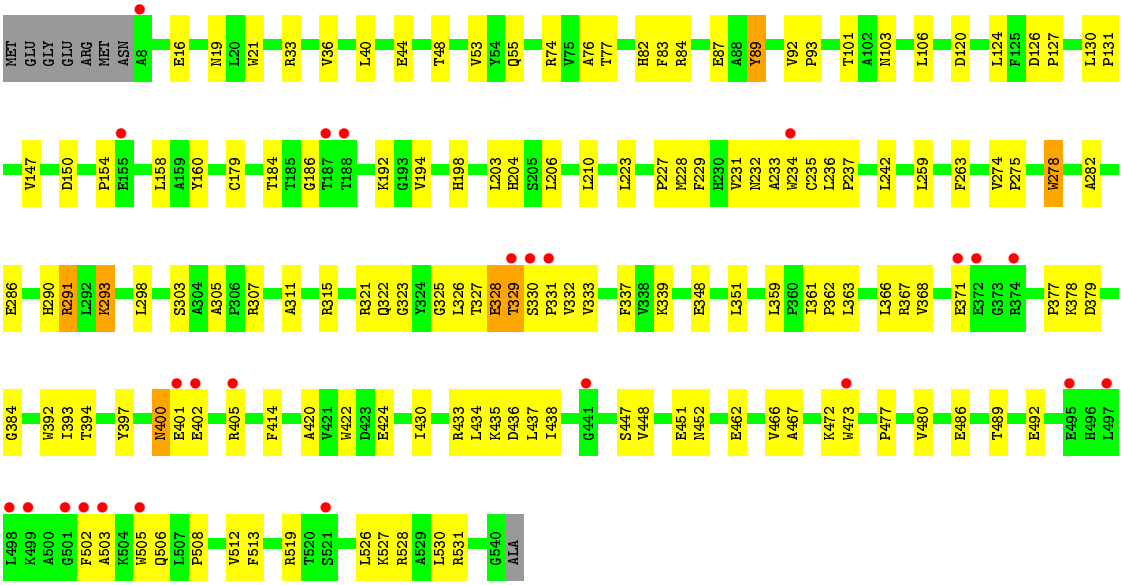
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	134	Total	O	0	0
			134	134		

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 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.

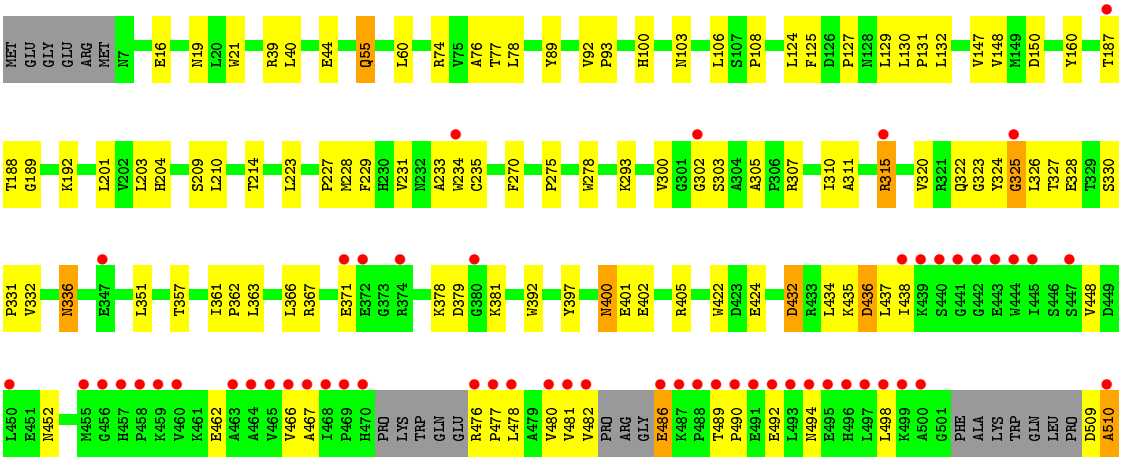
- Molecule 1: long chain fatty acid-CoA ligase

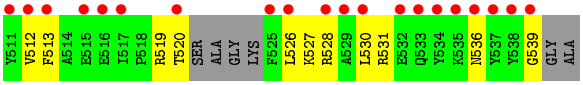
Chain A:



- Molecule 1: long chain fatty acid-CoA ligase

Chain B:




Y511
V512
F513
A514
E515
E516
I517
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 (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	8.51 (at 2.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.239 0.200 , 0.200	Depositor DCC
R_{free} test set	2446 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	36.6	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8431	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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:A:194:VAL:HG21	1:A:328:GLU:HA	1.80	0.64
1:B:489:THR:OG1	1:B:492:GLU:HG3	1.98	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:A:400:ASN:HD22	1:A:400:ASN:C	2.03	0.60
1:B:327:THR:HG23	1:B:330:SER:H	1.65	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:A:103:ASN:HB3	1:A:106:LEU:HG	1.90	0.53
1:A:19:ASN:HD22	1:A:21:TRP:H	1.55	0.53
1:B:39:ARG:HH11	1:B:39:ARG:HG3	1.73	0.53
1:B:462:GLU:CD	1:B:519:ARG:HH22	2.12	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:466:VAL:HG12	1:A:527:LYS:HD3	1.90	0.53
1:A:526:LEU:CD2	1:A:528:ARG:HB3	2.38	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: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:B:432:ASP:HA	1:B:448:VAL:CG2	2.39	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:19:ASN:ND2	1:A:21:TRP:H	2.08	0.50
1:A:329:THR:HG22	1:A:394:THR:H	1.75	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:A:361:ILE:HD11	1:A:392:TRP:CZ2	2.46	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:438:ILE:HG12	1:B:467:ALA:HB2	1.94	0.50
1:B:509:ASP:O	1:B:510:ALA:HB2	2.12	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:101:THR:HB	1:A:229:PHE:HA	1.95	0.49
1:A:433:ARG:HA	1:A:437:LEU:HB2	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:234:TRP:CH2	1:B:323:GLY:HA3	2.49	0.48
1:B:402:GLU:HG2	1:B:405:ARG:NH2	2.29	0.48
1:A:33:ARG:HD2	3:A:1078:HOH:O	2.14	0.47
1:A:124:LEU:CD2	1:A:147:VAL:HB	2.45	0.47
1:A:377:PRO:HB2	1:A:379:ASP:OD2	2.14	0.47
1:A:527:LYS:O	1:A:531:ARG:HG3	2.14	0.47
1:B:278:TRP:HA	1:B:278:TRP:HE3	1.78	0.47
1:A:378:LYS:HB2	1:A:424:GLU:OE2	2.14	0.47
1:B:124:LEU:CD2	1:B:147:VAL:HB	2.44	0.47
1:B:74:ARG:N	1:B:74:ARG:HD3	2.30	0.47
1:A:361:ILE:HD11	1:A:392:TRP:HZ2	1.80	0.47
1:B:466:VAL:HG12	1:B:527:LYS:HD3	1.97	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:A:82:HIS:HE1	1:A:126:ASP:OD1	1.98	0.46
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: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:B:39:ARG:NH1	1:B:39:ARG:HG3	2.30	0.46
1:A:438:ILE:CD1	1:A:477:PRO:HB3	2.45	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:366:LEU:HD23	1:A:367:ARG:N	2.31	0.46
1:B:478:LEU:HD11	1:B:512:VAL:HG23	1.96	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:A:130:LEU:HD21	1:A:154:PRO:HG2	1.99	0.43
1:B:125:PHE:CZ	1:B:148:VAL:HG22	2.53	0.43
1:B:361:ILE:HD11	1:B:392:TRP:CZ2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:ASP:OD1	1:B:381:LYS:N	2.45	0.43
1:B:361:ILE:HD11	1:B:392:TRP:HZ2	1.84	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:400:ASN:C	1:B:400:ASN:ND2	2.71	0.43
1:B:448:VAL:HG12	1:B:452:ASN:ND2	2.33	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:310:ILE:HG23	1:B:320:VAL:HB	2.00	0.42
1:B:490:PRO:O	1:B:494:ASN:ND2	2.53	0.42
1:B:19:ASN:ND2	1:B:21:TRP:HB3	2.34	0.42
1:A:298:LEU:HD23	1:A:298:LEU:C	2.39	0.42
1:A:307:ARG:NH2	1:A:348:GLU:O	2.52	0.42
1:A:36:VAL:HB	1:A:48:THR:HG23	2.02	0.42
1:B:476:ARG:HG2	1:B:476:ARG:HH11	1.84	0.42
1:B:77:THR:HA	1:B:124:LEU:O	2.19	0.42
1:A:486:GLU:O	1:A:486:GLU:HG3	2.18	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: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:A:293:LYS:HD2	1:A:293:LYS:H	1.84	0.42
1:B:204:HIS:HD2	1:B:392:TRP:CE2	2.38	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: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:502:PHE:HA	1:A:506:GLN:HE21	1.84	0.41
1:A:512:VAL:CG1	1:A:513:PHE:N	2.83	0.41
1:A:234:TRP:O	1:A:235:CYS:HB2	2.20	0.41
1:B:325:GLY:HA3	1:B:331:PRO:C	2.40	0.41
1:A:337:PHE:CE1	1:A:359:LEU:HD12	2.56	0.41
1:B:78:LEU:O	1:B:129:LEU:HD12	2.20	0.41
1:B:435:LYS:C	1:B:437:LEU:H	2.23	0.41
1:B:486:GLU:N	1:B:486:GLU:OE1	2.53	0.41
1:B:519:ARG:HB3	1:B:520:THR:H	1.69	0.41
1:A:326:LEU:C	1:A:328:GLU:N	2.74	0.41
1:A:329:THR:CB	1:A:394:THR:H	2.33	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:227:PRO:HB3	1:A:229:PHE:CE2	2.57	0.40
1:A:438:ILE:HG12	1:A:467:ALA:HB2	2.04	0.40
1:B:300:VAL:HG21	1:B:305:ALA:HB2	2.03	0.40
1:A:206:LEU:HD11	1:B:363:LEU:HD11	2.03	0.40
1:A:330:SER:HA	1:A:331:PRO:HD3	1.94	0.40
1:A:362:PRO:O	1:A:363:LEU:HB2	2.20	0.40
1:B:480:VAL:HG21	1:B:530:LEU:HD22	2.03	0.40
1:A:76:ALA:HB2	1:A:120:ASP:CG	2.42	0.40
1:A:204:HIS:NE2	1:A:332:VAL:HB	2.37	0.40
1:A:84:ARG:HH21	1:A:150:ASP:HA	1.86	0.40
1:B:328:GLU:H	1:B:328:GLU:CD	2.25	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	531/541 (98%)	510 (96%)	17 (3%)	4 (1%)	19	27
1	B	504/541 (93%)	484 (96%)	15 (3%)	5 (1%)	15	22
All	All	1035/1082 (96%)	994 (96%)	32 (3%)	9 (1%)	17	24

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%)	46	61
1	B	417/437 (95%)	406 (97%)	11 (3%)	46	61
All	All	848/874 (97%)	826 (97%)	22 (3%)	46	61

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	2.72	1 (33%)	3,17,17	3.12	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	-	-	3/6/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	CIT	O7-C3	4.34	1.49	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	CIT	C3-C2-C1	4.37	121.98	114.98
2	A	1001	CIT	C3-C4-C5	3.18	120.08	114.98

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	CIT	C1-C2-C3-O7
2	A	1001	CIT	C1-C2-C3-C4
2	A	1001	CIT	C1-C2-C3-C6

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^{th} 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^2)	Q<0.9
1	A	533/541 (98%)	0.13	25 (4%) 31 38	16, 36, 71, 81	0
1	B	514/541 (95%)	0.53	76 (14%) 2 2	17, 34, 112, 123	0
All	All	1047/1082 (96%)	0.33	101 (9%) 8 10	16, 35, 107, 123	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	511	TYR	8.4
1	B	500	ALA	7.8
1	B	468	ILE	7.8
1	A	329	THR	7.6
1	B	493	LEU	7.5
1	B	478	LEU	6.9
1	B	490	PRO	6.7
1	B	463	ALA	6.5
1	B	497	LEU	6.3
1	B	441	GLY	6.1
1	B	538	TYR	6.0
1	B	536	ASN	6.0
1	B	489	THR	5.9
1	B	440	SER	5.6
1	B	526	LEU	5.6
1	B	458	PRO	5.5
1	B	444	TRP	5.1
1	B	496	HIS	5.1
1	B	510	ALA	5.0
1	B	537	TYR	5.0
1	B	439	LYS	4.9
1	A	405	ARG	4.8
1	A	495	GLU	4.6
1	B	477	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	528	ARG	4.5
1	B	495	GLU	4.4
1	B	516	GLU	4.3
1	B	534	TYR	4.3
1	B	488	PRO	4.3
1	B	371	GLU	4.3
1	B	532	GLU	4.3
1	B	464	ALA	4.2
1	B	494	ASN	4.1
1	B	513	PHE	3.9
1	B	492	GLU	3.9
1	B	530	LEU	3.9
1	B	459	LYS	3.8
1	B	443	GLU	3.8
1	B	529	ALA	3.7
1	B	491	GLU	3.7
1	B	481	VAL	3.7
1	B	325	GLY	3.7
1	B	470	HIS	3.7
1	B	486	GLU	3.6
1	B	467	ALA	3.6
1	B	438	ILE	3.6
1	B	457	HIS	3.6
1	B	445	ILE	3.5
1	A	234	TRP	3.3
1	B	466	VAL	3.3
1	B	499	LYS	3.3
1	A	372	GLU	3.2
1	A	330	SER	3.2
1	A	401	GLU	3.2
1	B	469	PRO	3.2
1	B	482	VAL	3.2
1	A	502	PHE	3.2
1	A	8	ALA	3.2
1	A	501	GLY	3.1
1	B	460	VAL	3.1
1	A	505	TRP	3.0
1	B	187	THR	3.0
1	B	372	GLU	2.9
1	B	455	MET	2.9
1	B	517	ILE	2.8
1	A	371	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	456	GLY	2.8
1	B	487	LYS	2.8
1	B	447	SER	2.8
1	B	539	GLY	2.7
1	B	498	LEU	2.7
1	A	188	THR	2.7
1	B	442	GLY	2.7
1	B	465	VAL	2.7
1	B	315	ARG	2.7
1	B	476	ARG	2.6
1	A	441	GLY	2.6
1	B	515	GLU	2.6
1	B	520	THR	2.5
1	A	503	ALA	2.5
1	B	374	ARG	2.5
1	B	535	LYS	2.4
1	A	155	GLU	2.4
1	B	234	TRP	2.4
1	A	497	LEU	2.4
1	B	533	GLN	2.3
1	B	302	GLY	2.3
1	A	331	PRO	2.3
1	B	480	VAL	2.2
1	A	402	GLU	2.2
1	B	512	VAL	2.2
1	B	525	PHE	2.2
1	B	347	GLU	2.1
1	A	498	LEU	2.1
1	A	473	TRP	2.1
1	A	374	ARG	2.1
1	A	187	THR	2.1
1	A	521	SER	2.1
1	B	450	LEU	2.1
1	A	499	LYS	2.1
1	B	380	GLY	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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
2	CIT	A	1001	13/13	0.82	0.21	81,84,87,87	0

6.5 Other polymers (i)

There are no such residues in this entry.