



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 02:17 am BST

PDB ID : 1A6D
Title : THERMOSOME FROM T. ACIDOPHILUM
Authors : Ditzel, L.; Loewe, J.; Stock, D.; Stetter, K.-O.; Huber, H.; Huber, R.; Steinbacher, S.
Deposited on : 1998-02-24
Resolution : 2.60 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

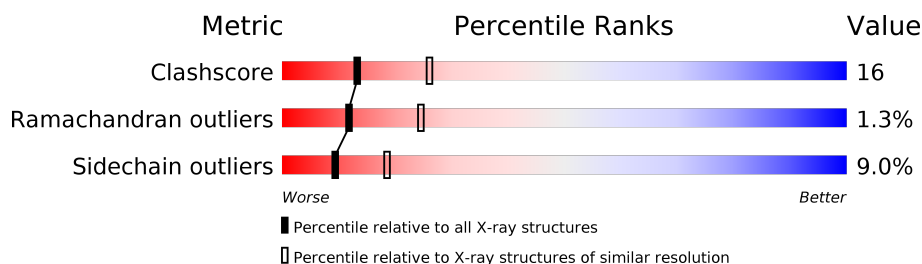
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	545	
2	B	543	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9324 atoms, of which 1742 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 THERMOSOME (ALPHA SUBUNIT).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	503	Total	C	H	N	O	S	884	0	0
			4668	2356	884	662	752	14			

- Molecule 2 is a protein called THERMOSOME (BETA SUBUNIT).

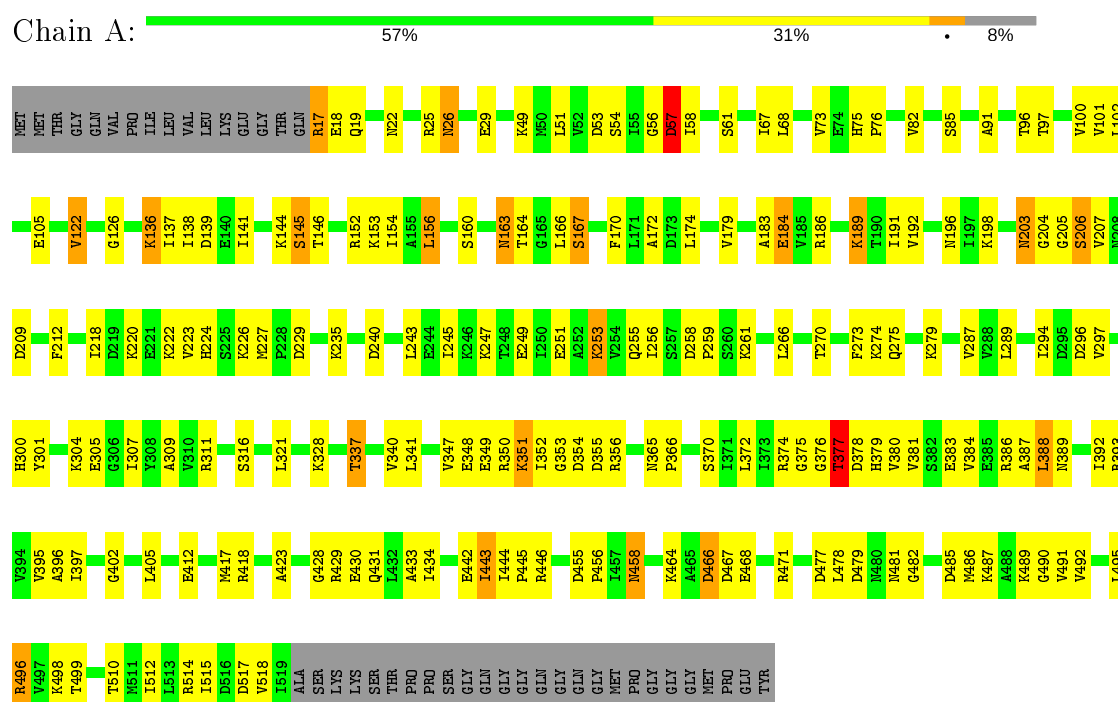
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	502	Total	C	H	N	O	S	858	0	0
			4656	2370	858	651	758	19			

3 Residue-property plots [i](#)

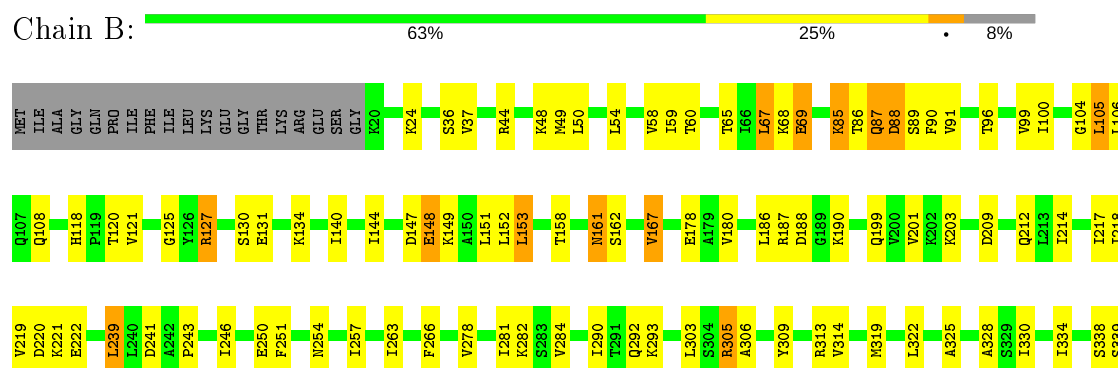
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: THERMOSOME (ALPHA SUBUNIT)



• Molecule 2: THERMOSOME (BETA SUBUNIT)



S340	E444	SER
R347	I445	GLU
Q350	P446	SER
V351	R447	SER
K352	I458	GLU
V353	L461	ASP
M358	L462	
T359	E467	
F360	H468	
V361	K473	
C364	I474	
K365	Y475	
N366	G476	
P367	I477	
K368	N478	
A369	G482	
V370	E483	
S371	I484	
G376	E485	
E384	D486	
F385	M487	
E386	V488	
R387	K489	
T390	N490	
D391	G491	
H394	V492	
V395	R497	
V396	I503	
L400	E504	
E401	T507	
D402	L514	
E415	V519	
R421	I520	
A424	A521	
Q425	THR	
K426	LYS	
R430	SER	
Q431	SER	
Q432	SER	
L433	SER	
A434	ASN	
K437	PRO	
A441	PRO	
I442	LYS	
E443	SER	
	GLY	
	SER	
	SER	

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	168.30 Å 168.30 Å 203.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	91.3 (8.00-2.60)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.215 , 0.298	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9324	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

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	0.52	0/3812	0.74	2/5139 (0.0%)
2	B	0.54	0/3834	0.73	1/5166 (0.0%)
All	All	0.53	0/7646	0.74	3/10305 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	ASP	N-CA-C	6.16	127.64	111.00
1	A	160	SER	N-CA-C	5.35	125.45	111.00
2	B	376	GLY	N-CA-C	-5.12	100.31	113.10

There are no chirality outliers.

There are no planarity outliers.

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	3784	884	3935	141	0
2	B	3798	858	3892	119	0
All	All	7582	1742	7827	249	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 16.

All (249) 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)
2:B:152:LEU:HD11	2:B:400:LEU:HD13	1.43	0.97
2:B:243:PRO:HD3	2:B:293:LYS:HD3	1.49	0.94
1:A:218:ILE:HD11	1:A:321:LEU:HD11	1.49	0.91
1:A:186:ARG:HG3	1:A:191:ILE:HD12	1.54	0.87
1:A:138:ILE:HD11	1:A:499:THR:CG2	2.07	0.84
1:A:51:LEU:HD23	2:B:520:ILE:HG13	1.60	0.82
1:A:136:LYS:N	1:A:136:LYS:HD3	2.00	0.76
1:A:138:ILE:HD11	1:A:499:THR:HG23	1.69	0.75
1:A:256:ILE:HG23	1:A:261:LYS:HB2	1.70	0.74
2:B:421:ARG:HG3	2:B:421:ARG:HH11	1.53	0.73
2:B:221:LYS:O	2:B:359:THR:HG22	1.88	0.73
1:A:51:LEU:HA	2:B:520:ILE:O	1.88	0.73
1:A:377:THR:O	1:A:378:ASP:HB3	1.90	0.72
1:A:275:GLN:O	1:A:279:LYS:HG2	1.90	0.71
1:A:486:MET:SD	1:A:491:VAL:HG21	2.31	0.71
2:B:152:LEU:HD11	2:B:400:LEU:CD1	2.19	0.71
2:B:58:VAL:HG11	2:B:69:GLU:HG2	1.73	0.70
1:A:412:GLU:OE2	1:A:498:LYS:HE3	1.91	0.69
2:B:85:LYS:HB3	2:B:87:GLN:HG2	1.72	0.69
1:A:163:ASN:HD21	2:B:127:ARG:HH22	1.40	0.69
2:B:503:ILE:O	2:B:507:THR:HG23	1.93	0.69
1:A:138:ILE:HD11	1:A:499:THR:HG22	1.74	0.69
1:A:163:ASN:ND2	2:B:127:ARG:HH12	1.92	0.68
1:A:397:ILE:HG23	1:A:496:ARG:HH21	1.59	0.67
1:A:154:ILE:HD13	1:A:492:VAL:HG23	1.75	0.67
1:A:218:ILE:CD1	1:A:321:LEU:HD11	2.24	0.67
1:A:258:ASP:HB3	1:A:261:LYS:HG2	1.76	0.66
1:A:204:GLY:HA3	1:A:374:ARG:CZ	2.26	0.66
1:A:17:ARG:HA	1:A:518:VAL:O	1.94	0.66
1:A:305:GLU:HB3	1:A:307:ILE:HD12	1.78	0.66
1:A:486:MET:HB3	1:A:491:VAL:HG22	1.77	0.66
2:B:425:GLN:OE1	2:B:426:LYS:HG3	1.96	0.66
2:B:239:LEU:HD22	2:B:328:ALA:HB3	1.77	0.66
2:B:424:ALA:HB1	2:B:432:GLN:HG3	1.78	0.65
1:A:164:THR:HG22	1:A:384:VAL:HG22	1.79	0.65
2:B:246:ILE:HD12	2:B:246:ILE:O	1.98	0.64
1:A:73:VAL:HG21	1:A:82:VAL:HG21	1.78	0.64
1:A:253:LYS:HE3	2:B:254:ASN:ND2	2.12	0.64
1:A:144:LYS:O	1:A:145:SER:HB2	1.99	0.63
2:B:152:LEU:CD1	2:B:400:LEU:HD13	2.23	0.63
2:B:68:LYS:HE3	2:B:85:LYS:HE3	1.81	0.62
1:A:405:LEU:HD12	1:A:498:LYS:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:458:ILE:O	2:B:462:LEU:HD13	1.99	0.62
2:B:309:TYR:OH	2:B:359:THR:HB	1.98	0.62
2:B:144:ILE:HG23	2:B:151:LEU:HD12	1.81	0.62
1:A:138:ILE:HA	1:A:141:ILE:HG12	1.80	0.62
1:A:348:GLU:CD	1:A:350:ARG:HH21	2.03	0.62
2:B:67:LEU:HD21	2:B:99:VAL:HG21	1.82	0.61
2:B:425:GLN:HA	2:B:432:GLN:NE2	2.16	0.60
1:A:204:GLY:HA3	1:A:374:ARG:NH1	2.16	0.60
2:B:104:GLY:O	2:B:108:GLN:HG2	2.02	0.59
1:A:351:LYS:HG2	1:A:355:ASP:O	2.02	0.59
2:B:490:ASN:N	2:B:490:ASN:HD22	2.01	0.59
2:B:96:THR:O	2:B:100:ILE:HG13	2.02	0.59
2:B:214:ILE:HG13	2:B:218:ILE:HD11	1.85	0.59
1:A:486:MET:SD	1:A:491:VAL:CG2	2.91	0.58
2:B:130:SER:HB2	2:B:507:THR:HG21	1.85	0.58
2:B:278:VAL:HG13	2:B:303:LEU:HD23	1.85	0.58
2:B:390:THR:O	2:B:394:HIS:HD2	1.87	0.58
1:A:510:THR:O	1:A:514:ARG:HG3	2.03	0.58
2:B:68:LYS:HE3	2:B:85:LYS:CE	2.34	0.58
1:A:222:LYS:HD2	1:A:227:MET:HB2	1.84	0.58
2:B:325:ALA:HA	2:B:366:ASN:HB3	1.86	0.58
2:B:121:VAL:HG11	2:B:430:ARG:HB3	1.87	0.57
1:A:56:GLY:O	1:A:57:ASP:HB2	2.04	0.57
2:B:445:ILE:HB	2:B:446:PRO:HD3	1.87	0.57
1:A:205:GLY:O	1:A:206:SER:HB3	2.05	0.56
2:B:65:THR:O	2:B:69:GLU:HB2	2.06	0.56
2:B:87:GLN:HA	2:B:90:PHE:CZ	2.41	0.55
2:B:85:LYS:O	2:B:90:PHE:HE1	1.90	0.55
1:A:270:THR:CG2	1:A:274:LYS:HE3	2.36	0.55
2:B:487:MET:CE	2:B:492:VAL:HG11	2.37	0.55
1:A:153:LYS:HE3	1:A:490:GLY:HA2	1.90	0.54
1:A:289:LEU:HD22	1:A:321:LEU:HD13	1.89	0.54
1:A:144:LYS:HD2	1:A:402:GLY:O	2.08	0.54
2:B:86:THR:O	2:B:86:THR:HG22	2.07	0.53
2:B:87:GLN:HA	2:B:90:PHE:CE1	2.43	0.53
1:A:491:VAL:O	1:A:491:VAL:HG23	2.09	0.53
1:A:203:ASN:O	1:A:376:GLY:HA2	2.09	0.53
2:B:222:GLU:HB2	2:B:350:GLN:OE1	2.09	0.53
1:A:294:ILE:HG13	1:A:311:ARG:HB3	1.89	0.53
1:A:218:ILE:HG22	1:A:220:LYS:HB2	1.92	0.52
1:A:97:THR:O	1:A:101:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:GLN:HG3	2:B:214:ILE:HD11	1.90	0.52
1:A:61:SER:HB2	1:A:386:ARG:NH1	2.25	0.52
2:B:421:ARG:HG3	2:B:421:ARG:NH1	2.18	0.52
1:A:444:ILE:HB	1:A:445:PRO:HD3	1.92	0.51
2:B:292:GLN:O	2:B:313:ARG:HA	2.11	0.51
2:B:134:LYS:CE	2:B:504:GLU:HG3	2.41	0.51
1:A:376:GLY:O	1:A:378:ASP:N	2.44	0.51
2:B:241:ASP:HB2	2:B:330:ILE:CG2	2.41	0.51
1:A:53:ASP:CG	1:A:54:SER:H	2.14	0.51
1:A:192:VAL:HG23	1:A:192:VAL:O	2.10	0.51
1:A:22:ASN:O	1:A:26:ASN:HB2	2.11	0.51
1:A:53:ASP:OD1	1:A:57:ASP:HA	2.09	0.51
2:B:290:ILE:HG23	2:B:314:VAL:HG21	1.93	0.51
2:B:475:TYR:HA	2:B:485:GLU:O	2.11	0.51
2:B:140:ILE:HD13	2:B:415:GLU:HG2	1.92	0.51
1:A:25:ARG:O	1:A:29:GLU:HG2	2.11	0.50
2:B:217:ILE:O	2:B:361:VAL:HG12	2.11	0.50
2:B:50:LEU:HB2	2:B:58:VAL:HG13	1.94	0.50
1:A:222:LYS:HG2	1:A:349:GLU:OE2	2.11	0.50
2:B:118:HIS:HD2	2:B:120:THR:HB	1.76	0.50
2:B:282:LYS:HD3	2:B:306:ALA:HB1	1.92	0.50
2:B:201:VAL:HG11	2:B:358:MET:HE1	1.93	0.49
2:B:54:LEU:HD12	2:B:54:LEU:H	1.76	0.49
1:A:423:ALA:O	1:A:431:GLN:HG3	2.12	0.49
1:A:126:GLY:HA3	1:A:433:ALA:HB3	1.93	0.49
2:B:54:LEU:HD12	2:B:54:LEU:N	2.26	0.49
1:A:247:LYS:HE3	2:B:251:PHE:HA	1.95	0.49
1:A:137:ILE:HD13	1:A:418:ARG:HD2	1.95	0.49
2:B:220:ASP:O	2:B:221:LYS:HG2	2.12	0.49
2:B:489:LYS:HD3	2:B:489:LYS:C	2.34	0.49
2:B:281:ILE:O	2:B:284:VAL:HG12	2.13	0.49
1:A:235:LYS:HE2	1:A:341:LEU:HD12	1.94	0.48
1:A:352:ILE:HG21	1:A:372:LEU:HD21	1.95	0.48
2:B:118:HIS:HD2	2:B:120:THR:CB	2.26	0.48
2:B:186:LEU:HA	2:B:190:LYS:O	2.13	0.48
1:A:443:ILE:O	1:A:443:ILE:HD13	2.14	0.48
2:B:334:ILE:HD12	2:B:334:ILE:H	1.79	0.48
1:A:105:GLU:HG2	1:A:443:ILE:HB	1.95	0.48
1:A:405:LEU:CD1	1:A:498:LYS:HG3	2.43	0.48
1:A:53:ASP:OD1	1:A:54:SER:N	2.47	0.48
1:A:192:VAL:CG2	1:A:396:ALA:HB1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:LEU:O	1:A:392:ILE:HG13	2.14	0.48
1:A:389:ASN:O	1:A:393:ARG:HG3	2.13	0.47
2:B:284:VAL:CG2	2:B:339:SER:N	2.77	0.47
1:A:163:ASN:HD21	2:B:127:ARG:NH2	2.08	0.47
1:A:184:GLU:OE1	1:A:191:ILE:HB	2.14	0.47
1:A:245:ILE:HG12	1:A:273:PHE:CZ	2.49	0.47
1:A:477:ASP:N	1:A:482:GLY:O	2.45	0.47
1:A:192:VAL:HG21	1:A:396:ALA:HB1	1.96	0.47
1:A:287:VAL:HG21	1:A:347:VAL:HG21	1.95	0.47
1:A:351:LYS:NZ	1:A:353:GLY:O	2.47	0.47
1:A:466:ASP:OD2	1:A:471:ARG:HD3	2.15	0.47
1:A:183:ALA:HA	1:A:192:VAL:HG12	1.96	0.47
2:B:149:LYS:O	2:B:153:LEU:HD22	2.15	0.47
1:A:206:SER:HB3	1:A:209:ASP:OD2	2.14	0.47
1:A:337:THR:O	1:A:340:VAL:HG22	2.15	0.47
1:A:247:LYS:HA	2:B:251:PHE:CZ	2.50	0.47
2:B:366:ASN:ND2	2:B:368:LYS:H	2.13	0.46
1:A:397:ILE:HG23	1:A:496:ARG:HE	1.80	0.46
2:B:476:GLY:O	2:B:484:ILE:HA	2.15	0.46
1:A:377:THR:O	1:A:378:ASP:CB	2.63	0.46
1:A:49:LYS:HG3	1:A:67:ILE:HD13	1.96	0.46
2:B:37:VAL:CG1	2:B:96:THR:HG23	2.45	0.46
1:A:179:VAL:HG21	1:A:395:VAL:HG12	1.98	0.46
2:B:241:ASP:HB2	2:B:330:ILE:HG22	1.96	0.46
2:B:347:ARG:CB	2:B:347:ARG:HH11	2.28	0.46
2:B:384:GLU:OE1	2:B:387:ARG:NH1	2.49	0.46
1:A:183:ALA:CB	1:A:192:VAL:HG12	2.45	0.46
1:A:91:ALA:HA	1:A:96:THR:OG1	2.15	0.46
1:A:430:GLU:O	1:A:434:ILE:HG13	2.15	0.46
1:A:163:ASN:ND2	2:B:127:ARG:HH22	2.12	0.46
2:B:60:THR:HB	2:B:387:ARG:NH1	2.30	0.46
2:B:147:ASP:HB3	2:B:151:LEU:HG	1.98	0.45
2:B:188:ASP:C	2:B:190:LYS:H	2.19	0.45
2:B:86:THR:O	2:B:88:ASP:N	2.49	0.45
2:B:219:VAL:HG21	2:B:322:LEU:HD11	1.98	0.45
1:A:19:GLN:HG2	1:A:517:ASP:CG	2.36	0.45
2:B:402:ASP:OD2	2:B:497:ARG:HB2	2.17	0.45
1:A:205:GLY:O	1:A:206:SER:CB	2.65	0.45
1:A:397:ILE:HG23	1:A:496:ARG:NH2	2.31	0.45
1:A:122:VAL:HG21	1:A:429:ARG:HB3	1.98	0.45
1:A:486:MET:HB3	1:A:491:VAL:CG2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LYS:HE3	1:A:490:GLY:CA	2.47	0.45
1:A:270:THR:HG22	1:A:274:LYS:HE3	1.99	0.44
2:B:433:LEU:O	2:B:437:LYS:HG2	2.18	0.44
1:A:156:LEU:HD22	1:A:172:ALA:CB	2.47	0.44
1:A:207:VAL:HA	1:A:374:ARG:O	2.18	0.44
2:B:325:ALA:O	2:B:364:CYS:HB3	2.18	0.44
2:B:322:LEU:CD2	2:B:361:VAL:HG11	2.46	0.44
1:A:297:VAL:CG1	1:A:301:TYR:HE2	2.30	0.44
1:A:351:LYS:HG3	1:A:356:ARG:HG2	1.99	0.44
1:A:186:ARG:HG3	1:A:191:ILE:CD1	2.38	0.44
1:A:405:LEU:HD21	1:A:495:LEU:HD13	1.99	0.44
2:B:199:GLN:O	2:B:371:SER:HA	2.18	0.44
2:B:118:HIS:CD2	2:B:120:THR:H	2.35	0.44
1:A:224:HIS:CE1	1:A:226:LYS:HB2	2.53	0.44
1:A:255:GLN:OE1	2:B:254:ASN:HB2	2.17	0.44
1:A:144:LYS:O	1:A:145:SER:CB	2.65	0.43
2:B:105:LEU:HD13	2:B:441:ALA:CB	2.47	0.43
1:A:259:PRO:HA	2:B:266:PHE:CE1	2.53	0.43
1:A:18:GLU:O	1:A:517:ASP:HA	2.18	0.43
1:A:328:LYS:HB2	1:A:340:VAL:HB	1.99	0.43
1:A:455:ASP:OD2	1:A:458:ASN:HB2	2.18	0.43
1:A:417:MET:SD	1:A:468:GLU:HG3	2.58	0.43
1:A:57:ASP:HB3	1:A:58:ILE:H	1.69	0.43
2:B:366:ASN:HD22	2:B:366:ASN:C	2.21	0.43
2:B:203:LYS:HG2	2:B:353:VAL:HG12	2.00	0.43
2:B:437:LYS:HA	2:B:437:LYS:HD3	1.76	0.43
2:B:467:GLU:HG3	2:B:484:ILE:HG21	2.01	0.43
1:A:223:VAL:HG22	1:A:309:ALA:O	2.18	0.43
1:A:479:ASP:C	1:A:481:ASN:H	2.21	0.43
2:B:180:VAL:HG21	2:B:396:VAL:HG22	2.00	0.43
2:B:86:THR:CG2	2:B:86:THR:O	2.67	0.43
2:B:158:THR:O	2:B:161:ASN:HB2	2.19	0.42
1:A:174:LEU:HD22	1:A:212:PHE:HB2	2.01	0.42
1:A:17:ARG:HH21	1:A:19:GLN:HG3	1.84	0.42
1:A:297:VAL:O	1:A:300:HIS:HB3	2.19	0.42
1:A:207:VAL:C	1:A:209:ASP:N	2.72	0.42
2:B:503:ILE:O	2:B:507:THR:CG2	2.66	0.42
1:A:365:ASN:HA	1:A:366:PRO:HD3	1.79	0.42
1:A:186:ARG:HB2	1:A:189:LYS:HD2	2.02	0.42
2:B:443:GLU:O	2:B:447:ARG:HG3	2.19	0.42
2:B:130:SER:CB	2:B:507:THR:HG21	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:HIS:HA	1:A:76:PRO:HD3	1.92	0.42
2:B:284:VAL:HG21	2:B:338:SER:C	2.40	0.42
2:B:50:LEU:HB2	2:B:58:VAL:CG1	2.49	0.42
1:A:446:ARG:HG3	1:A:456:PRO:HB3	2.02	0.42
2:B:290:ILE:CG2	2:B:314:VAL:HG21	2.50	0.42
1:A:274:LYS:HE2	1:A:301:TYR:CZ	2.55	0.41
1:A:380:VAL:HG13	1:A:381:VAL:N	2.34	0.41
1:A:405:LEU:HD11	1:A:495:LEU:HD12	2.02	0.41
1:A:186:ARG:HB2	1:A:189:LYS:HE2	2.02	0.41
2:B:44:ARG:HG2	2:B:44:ARG:HH11	1.85	0.41
2:B:89:SER:HB3	2:B:91:VAL:HG23	2.02	0.41
1:A:102:LEU:HA	1:A:102:LEU:HD12	1.91	0.41
2:B:67:LEU:HD12	2:B:67:LEU:HA	1.91	0.41
1:A:53:ASP:CG	1:A:54:SER:N	2.74	0.41
2:B:487:MET:SD	2:B:492:VAL:CG1	3.09	0.41
1:A:198:LYS:O	1:A:370:SER:HA	2.20	0.41
2:B:478:ASN:O	2:B:482:GLY:N	2.49	0.41
2:B:484:ILE:N	2:B:484:ILE:HD12	2.35	0.41
2:B:284:VAL:HG21	2:B:339:SER:N	2.36	0.41
1:A:68:LEU:HD11	1:A:100:VAL:HG21	2.02	0.41
1:A:489:LYS:HB3	1:A:489:LYS:HE2	1.78	0.41
2:B:292:GLN:HE21	2:B:319:MET:HG2	1.86	0.41
2:B:48:LYS:O	2:B:59:ILE:HA	2.20	0.41
2:B:468:HIS:HE1	2:B:473:LYS:O	2.04	0.41
1:A:167:SER:O	1:A:170:PHE:HB3	2.21	0.41
2:B:125:GLY:HA3	2:B:434:ALA:HB3	2.02	0.41
1:A:206:SER:O	1:A:207:VAL:HB	2.21	0.41
1:A:442:GLU:O	1:A:445:PRO:HD2	2.21	0.41
1:A:512:ILE:HA	1:A:515:ILE:HD12	2.02	0.41
2:B:257:ILE:HG21	2:B:263:ILE:HG13	2.03	0.41
1:A:351:LYS:HB3	1:A:351:LYS:HE2	1.77	0.41
1:A:485:ASP:OD2	1:A:487:LYS:HB3	2.21	0.41
2:B:487:MET:HE3	2:B:492:VAL:HG11	2.02	0.41
2:B:347:ARG:HB2	2:B:347:ARG:HH11	1.85	0.40
1:A:479:ASP:C	1:A:481:ASN:N	2.74	0.40
1:A:485:ASP:OD1	1:A:487:LYS:HB3	2.22	0.40
1:A:68:LEU:HB2	1:A:85:SER:OG	2.21	0.40
1:A:186:ARG:HB2	1:A:189:LYS:CE	2.51	0.40
2:B:305:ARG:HA	2:B:305:ARG:NE	2.36	0.40
1:A:383:GLU:O	1:A:387:ALA:N	2.51	0.40
1:A:196:ASN:HA	1:A:196:ASN:HD22	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:485:GLU:OE1	2:B:490:ASN:OD1	2.39	0.40
2:B:36:SER:O	2:B:48:LYS:HE3	2.21	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	501/545 (92%)	464 (93%)	29 (6%)	8 (2%)	9	19
2	B	500/543 (92%)	477 (95%)	18 (4%)	5 (1%)	15	32
All	All	1001/1088 (92%)	941 (94%)	47 (5%)	13 (1%)	12	24

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ASP
1	A	145	SER
1	A	206	SER
1	A	377	THR
1	A	428	GLY
2	B	87	GLN
2	B	187	ARG
2	B	85	LYS
1	A	167	SER
1	A	203	ASN
1	A	375	GLY
2	B	167	VAL
2	B	148	GLU

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	411/442 (93%)	375 (91%)	36 (9%)	10	19
2	B	410/446 (92%)	372 (91%)	38 (9%)	9	17
All	All	821/888 (92%)	747 (91%)	74 (9%)	9	18

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	26	ASN
1	A	57	ASP
1	A	122	VAL
1	A	136	LYS
1	A	139	ASP
1	A	146	THR
1	A	152	ARG
1	A	156	LEU
1	A	163	ASN
1	A	166	LEU
1	A	184	GLU
1	A	189	LYS
1	A	229	ASP
1	A	240	ASP
1	A	243	LEU
1	A	249	GLU
1	A	251	GLU
1	A	253	LYS
1	A	266	LEU
1	A	296	ASP
1	A	304	LYS
1	A	316	SER
1	A	337	THR
1	A	351	LYS
1	A	354	ASP
1	A	377	THR

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Mol	Chain	Res	Type
1	A	379	HIS
1	A	388	LEU
1	A	443	ILE
1	A	458	ASN
1	A	464	LYS
1	A	466	ASP
1	A	467	ASP
1	A	478	LEU
1	A	496	ARG
2	B	24	LYS
2	B	49	MET
2	B	67	LEU
2	B	69	GLU
2	B	88	ASP
2	B	105	LEU
2	B	106	LEU
2	B	127	ARG
2	B	131	GLU
2	B	148	GLU
2	B	153	LEU
2	B	161	ASN
2	B	162	SER
2	B	167	VAL
2	B	178	GLU
2	B	209	ASP
2	B	239	LEU
2	B	250	GLU
2	B	305	ARG
2	B	340	SER
2	B	347	ARG
2	B	351	VAL
2	B	359	THR
2	B	366	ASN
2	B	370	VAL
2	B	386	GLU
2	B	391	ASP
2	B	396	VAL
2	B	421	ARG
2	B	425	GLN
2	B	461	LEU
2	B	487	MET
2	B	490	ASN

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Mol	Chain	Res	Type
2	B	492	VAL
2	B	503	ILE
2	B	507	THR
2	B	514	LEU
2	B	519	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	109	GLN
1	A	125	ASN
1	A	132	ASN
1	A	163	ASN
1	A	180	ASN
1	A	196	ASN
1	A	233	ASN
1	A	267	ASN
1	A	299	GLN
1	A	365	ASN
1	A	424	ASN
1	A	451	ASN
1	A	480	ASN
2	B	26	ASN
2	B	35	ASN
2	B	108	GLN
2	B	118	HIS
2	B	161	ASN
2	B	254	ASN
2	B	292	GLN
2	B	300	GLN
2	B	301	HIS
2	B	366	ASN
2	B	394	HIS
2	B	432	GLN
2	B	472	ASN
2	B	490	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.