



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:44 AM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

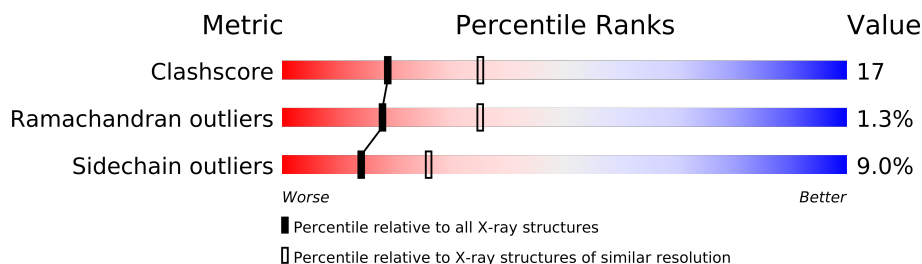
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 deuterium.

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			

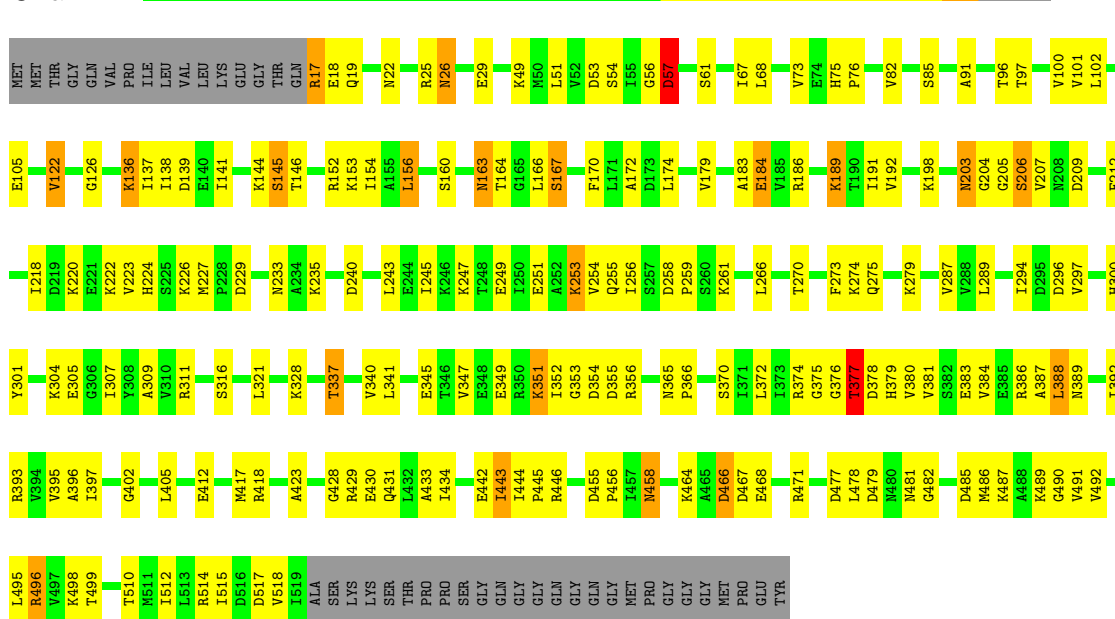
3 Residue-property plots

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.

Note EDS was not executed.

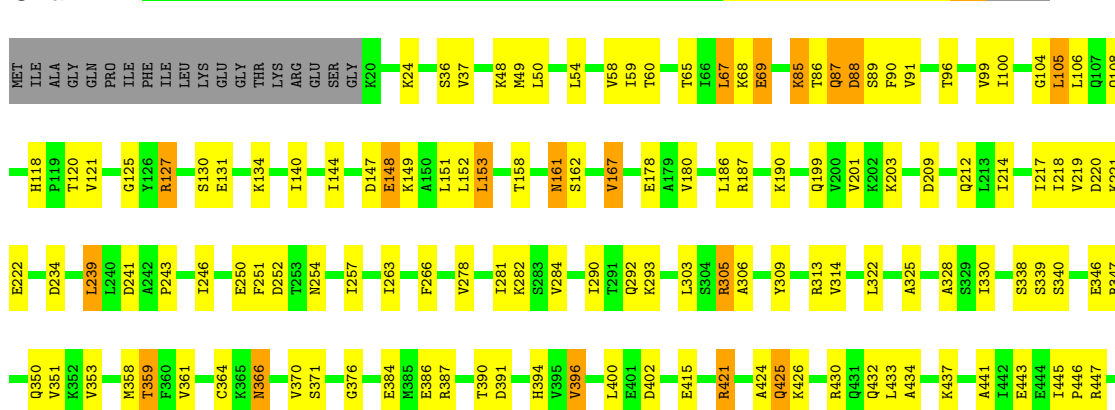
• Molecule 1: THERMOSOME (ALPHA SUBUNIT)

Chain A:



• Molecule 2: THERMOSOME (BETA SUBUNIT)

Chain B:



I458	
I461	
I462	
E467	
H468	
K473	
T474	
Y475	
G476	
T477	
N478	
G482	
E483	
I484	
E485	
D486	
N487	
W488	
K489	
N490	
G491	
W492	
R497	
I503	
E504	
T507	
L514	
V519	
I520	
A521	
THR	
LYS	
SER	
SER	
SER	
SER	
SER	
SER	
ASN	
PRO	
PRO	
LYS	
SER	
GLY	
SER	
SER	
GLU	
SER	
SER	
GLU	

ASP

4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	168.30Å 168.30Å 203.40Å 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

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	0.52	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3784	884	3050	132	0
2	B	3798	858	3034	106	0
All	All	7582	1742	6084	229	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (229) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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: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
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: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:486:MET:HB3	1:A:491:VAL:HG22	1.77	0.66
1:A:305:GLU:HB3	1:A:307:ILE:HD12	1.78	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:214:ILE:HG13	2:B:218:ILE:HD11	1.85	0.59
2:B:96:THR:O	2:B:100:ILE:HG13	2.02	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:390:THR:O	2:B:394:HIS:HD2	1.87	0.58
2:B:278:VAL:HG13	2:B:303:LEU:HD23	1.85	0.58
2:B:68:LYS:HE3	2:B:85:LYS:CE	2.34	0.58
1:A:510:THR:O	1:A:514:ARG:HG3	2.03	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:421:ARG:NH1	2:B:421:ARG:HG3	2.18	0.57
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:289:LEU:HD22	1:A:321:LEU:HD13	1.89	0.54
1:A:153:LYS:HE3	1:A:490:GLY:HA2	1.90	0.54
1:A:144:LYS:HD2	1:A:402:GLY:O	2.08	0.54
2:B:87:GLN:HA	2:B:90:PHE:CE1	2.43	0.53
2:B:86:THR:O	2:B:86:THR:HG22	2.07	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
2:B:212:GLN:HG3	2:B:214:ILE:HD11	1.90	0.52
1:A:97:THR:O	1:A:101:VAL:HG23	2.09	0.52
1:A:61:SER:HB2	1:A:386:ARG:NH1	2.25	0.52
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:444:ILE:HB	1:A:445:PRO:HD3	1.92	0.51
1:A:376:GLY:O	1:A:378:ASP:N	2.44	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:241:ASP:HB2	2:B:330:ILE:CG2	2.41	0.51
1:A:53:ASP:OD1	1:A:57:ASP:HA	2.09	0.51
2:B:475:TYR:HA	2:B:485:GLU:O	2.11	0.51
1:A:192:VAL:HG23	1:A:192:VAL:O	2.10	0.51
2:B:290:ILE:HG23	2:B:314:VAL:HG21	1.93	0.51
1:A:22:ASN:O	1:A:26:ASN:HB2	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:282:LYS:HD3	2:B:306:ALA:HB1	1.92	0.50
2:B:118:HIS:HD2	2:B:120:THR:HB	1.76	0.50
2:B:201:VAL:HG11	2:B:358:MET:HE1	1.93	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
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
1:A:137:ILE:HD13	1:A:418:ARG:HD2	1.95	0.49
1:A:477:ASP:N	1:A:482:GLY:O	2.45	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
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
1:A:388:LEU:O	1:A:392:ILE:HG13	2.14	0.48
2:B:284:VAL:CG2	2:B:339:SER:N	2.77	0.47
1:A:389:ASN:O	1:A:393:ARG:HG3	2.13	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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
2:B:37:VAL:CG1	2:B:96:THR:HG23	2.45	0.46
1:A:49:LYS:HG3	1:A:67:ILE:HD13	1.96	0.46
2:B:241:ASP:HB2	2:B:330:ILE:HG22	1.96	0.46
1:A:179:VAL:HG21	1:A:395:VAL:HG12	1.98	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
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: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
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:478:ASN:O	2:B:482:GLY:N	2.49	0.44
2:B:433:LEU:O	2:B:437:LYS:HG2	2.18	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
1:A:156:LEU:HD22	1:A:172:ALA:CB	2.47	0.44
2:B:322:LEU:CD2	2:B:361:VAL:HG11	2.46	0.44
1:A:351:LYS:HG3	1:A:356:ARG:HG2	1.99	0.44
1:A:297:VAL:CG1	1:A:301:TYR:HE2	2.30	0.44
1:A:383:GLU:O	1:A:387:ALA:N	2.51	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
1:A:255:GLN:OE1	2:B:254:ASN:HB2	2.17	0.44
1:A:224:HIS:CE1	1:A:226:LYS:HB2	2.53	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:259:PRO:HA	2:B:266:PHE:CE1	2.53	0.43
1:A:328:LYS:HB2	1:A:340:VAL:HB	1.99	0.43
1:A:18:GLU:O	1:A:517:ASP:HA	2.18	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:233:ASN:N	1:A:345:GLU:O	2.50	0.43
2:B:203:LYS:HG2	2:B:353:VAL:HG12	2.00	0.43
2:B:467:GLU:HG3	2:B:484:ILE:HG21	2.01	0.43
2:B:437:LYS:HA	2:B:437:LYS:HD3	1.76	0.43
1:A:223:VAL:HG22	1:A:309:ALA:O	2.18	0.43
2:B:86:THR:CG2	2:B:86:THR:O	2.67	0.43
2:B:180:VAL:HG21	2:B:396:VAL:HG22	2.00	0.43
2:B:158:THR:O	2:B:161:ASN:HB2	2.19	0.42
1:A:297:VAL:O	1:A:300:HIS:HB3	2.19	0.42
1:A:174:LEU:HD22	1:A:212:PHE:HB2	2.01	0.42
2:B:503:ILE:O	2:B:507:THR:CG2	2.66	0.42
1:A:207:VAL:C	1:A:209:ASP:N	2.72	0.42
1:A:254:VAL:N	2:B:252:ASP:O	2.52	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
1:A:75:HIS:HA	1:A:76:PRO:HD3	1.92	0.42
2:B:50:LEU:HB2	2:B:58:VAL:CG1	2.49	0.42
2:B:284:VAL:HG21	2:B:338:SER:C	2.40	0.42
2:B:290:ILE:CG2	2:B:314:VAL:HG21	2.50	0.42
2:B:234:ASP:N	2:B:346:GLU:O	2.53	0.42
1:A:446:ARG:HG3	1:A:456:PRO:HB3	2.02	0.42
1:A:405:LEU:HD11	1:A:495:LEU:HD12	2.02	0.41
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:186:ARG:HB2	1:A:189:LYS:HE2	2.02	0.41
2:B:89:SER:HB3	2:B:91:VAL:HG23	2.02	0.41
2:B:67:LEU:HD12	2:B:67:LEU:HA	1.91	0.41
1:A:102:LEU:HA	1:A:102:LEU:HD12	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
2:B:484:ILE:N	2:B:484:ILE:HD12	2.35	0.41
1:A:198:LYS:O	1:A:370:SER:HA	2.20	0.41
2:B:284:VAL:HG21	2:B:339:SER:N	2.36	0.41
2:B:48:LYS:O	2:B:59:ILE:HA	2.20	0.41
1:A:68:LEU:HD11	1:A:100:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:489:LYS:HB3	1:A:489:LYS:HE2	1.78	0.41
2:B:468:HIS:HE1	2:B:473:LYS:O	2.04	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: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: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
2:B:487:MET:HE3	2:B:492:VAL:HG11	2.02	0.41
1:A:485:ASP:OD2	1:A:487:LYS:HB3	2.21	0.41
1:A:163:ASN:ND2	2:B:127:ARG:NH1	2.69	0.41
1:A:68:LEU:HB2	1:A:85:SER:OG	2.21	0.40
1:A:485:ASP:OD1	1:A:487:LYS:HB3	2.22	0.40
1:A:479:ASP:C	1:A:481:ASN:N	2.74	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
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

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	501/545 (92%)	464 (93%)	29 (6%)	8 (2%)	14	28
2	B	500/543 (92%)	477 (95%)	18 (4%)	5 (1%)	22	45
All	All	1001/1088 (92%)	941 (94%)	47 (5%)	13 (1%)	18	35

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ASP

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Mol	Chain	Res	Type
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%)	14	27
2	B	410/446 (92%)	372 (91%)	38 (9%)	13	24
All	All	821/888 (92%)	747 (91%)	74 (9%)	14	26

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	163	ASN
1	A	379	HIS
2	B	118	HIS
2	B	254	ASN
2	B	300	GLN
2	B	301	HIS
2	B	394	HIS
2	B	431	GLN
2	B	432	GLN
2	B	490	ASN
2	B	501	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.