



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:47 AM UTC

PDB ID : 1A6D / pdb_00001a6d
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

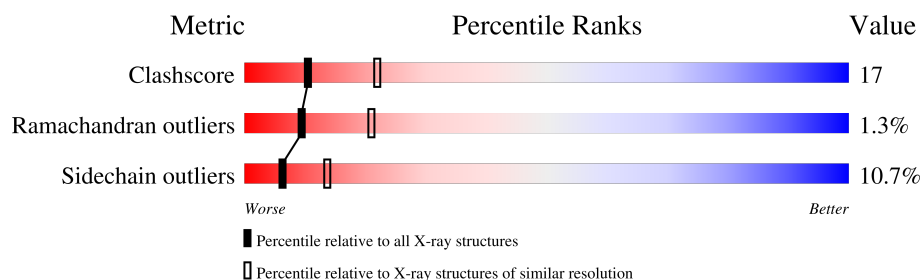
1 Overall quality at a glance

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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (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 of 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.

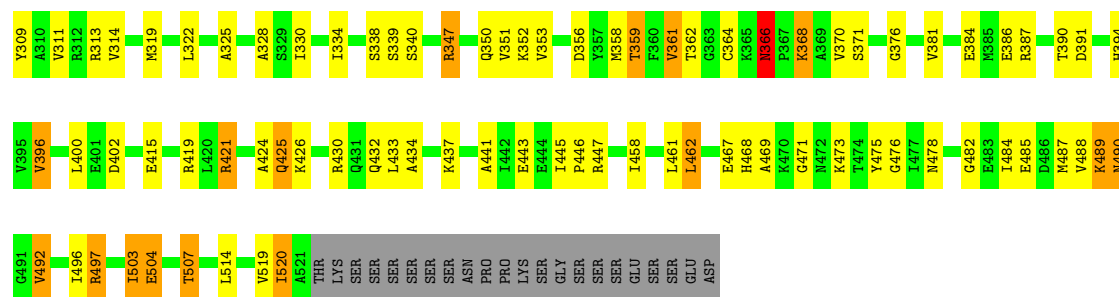
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- 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			



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	168.30Å 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	0.70	1/3812 (0.0%)	1.11	23/5139 (0.4%)
2	B	0.73	0/3834	1.10	18/5166 (0.3%)
All	All	0.71	1/7646 (0.0%)	1.10	41/10305 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	MET	SD-CE	-6.93	1.62	1.79

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	SER	N-CA-C	11.83	125.45	111.02
2	B	42	GLY	CA-C-N	10.47	130.24	119.56
2	B	42	GLY	C-N-CA	10.47	130.24	119.56
2	B	189	GLY	N-CA-C	-8.55	103.99	115.36
1	A	62	ASN	N-CA-C	-8.08	103.62	113.97
2	B	356	ASP	N-CA-C	8.00	121.09	110.53
1	A	57	ASP	N-CA-C	7.91	127.64	110.80
1	A	43	GLY	CA-C-N	7.71	127.77	119.28
1	A	43	GLY	C-N-CA	7.71	127.77	119.28
2	B	376	GLY	N-CA-C	-7.11	100.31	110.91
1	A	365	ASN	CA-C-N	7.07	126.70	119.56
1	A	365	ASN	C-N-CA	7.07	126.70	119.56
2	B	121	VAL	N-CA-C	-6.78	104.05	110.42
1	A	58	ILE	N-CA-C	6.75	118.39	109.21
1	A	223	VAL	N-CA-C	6.55	119.24	111.05
2	B	368	LYS	N-CA-C	-6.50	102.47	110.65
1	A	236	ILE	N-CA-C	6.30	117.87	108.23
2	B	237	ILE	N-CA-C	5.91	117.26	108.23
2	B	381	VAL	N-CA-C	-5.83	106.03	111.45
2	B	299	ALA	N-CA-C	-5.76	105.08	111.36
1	A	324	ALA	N-CA-C	5.70	117.57	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	LEU	N-CA-C	5.60	117.82	109.59
2	B	169	LYS	N-CA-C	5.59	117.37	111.28
1	A	139	ASP	N-CA-C	-5.56	105.37	111.82
1	A	455	ASP	CA-C-N	5.43	124.61	118.97
1	A	455	ASP	C-N-CA	5.43	124.61	118.97
1	A	203	ASN	N-CA-C	5.42	122.35	110.80
1	A	361	MET	N-CA-C	5.41	118.39	109.85
1	A	397	ILE	CB-CA-C	-5.39	105.07	111.97
2	B	497	ARG	N-CA-C	5.36	117.12	111.28
2	B	38	ARG	N-CA-C	5.34	117.52	111.11
2	B	469	ALA	N-CA-C	-5.33	105.55	111.36
2	B	366	ASN	CA-C-N	5.27	125.73	120.04
2	B	366	ASN	C-N-CA	5.27	125.73	120.04
1	A	469	LYS	N-CA-C	-5.21	106.89	113.20
1	A	435	GLU	N-CA-C	-5.18	105.70	112.23
1	A	208	ASN	N-CA-C	-5.16	106.67	112.87
2	B	61	ASN	N-CA-C	-5.14	107.04	113.72
1	A	75	HIS	CA-C-N	5.08	124.25	118.97
1	A	75	HIS	C-N-CA	5.08	124.25	118.97
2	B	471	GLY	N-CA-C	5.04	122.66	114.90

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	3784	884	3935	149	0
2	B	3798	858	3892	123	0
All	All	7582	1742	7827	261	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 17.

All (261) 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:511:LEU:HD23	2:B:520:ILE:HG13	1.60	0.82
1:A:136:LYS:HD3	1:A:136:LYS:N	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:511: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
2:B:201:VAL:HG11	2:B:358:MET:HE1	1.74	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:348:GLU:CD	1:A:350:ARG:HH21	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:53:ASP:CG	1:A:54:SER:H	2.14	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:489:LYS:HD3	2:B:489:LYS:C	2.34	0.53
2:B:86:THR:HG22	2:B:86:THR:O	2.07	0.53
2:B:87:GLN:HA	2:B:90:PHE:CE1	2.43	0.53
1:A:491:VAL:HG23	1:A:491:VAL:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:134:LYS:CE	2:B:504:GLU:HG3	2.41	0.51
2:B:292:GLN:O	2:B:313:ARG:HA	2.11	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: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
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
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
2:B:188:ASP:C	2:B:190:LYS:H	2.19	0.50
1:A:222:LYS:HG2	1:A:349:GLU:OE2	2.11	0.50
1:A:19:GLN:HG2	1:A:517:ASP:CG	2.36	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: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
2:B:487:MET:HE3	2:B:492:VAL:HG11	1.94	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: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:HD13	1:A:443:ILE:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:389:ASN:O	1:A:393:ARG:HG3	2.13	0.47
1:A:479:ASP:C	1:A:481:ASN:H	2.21	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
2:B:366:ASN:HD22	2:B:366:ASN:C	2.21	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:207:VAL:C	1:A:209:ASP:N	2.72	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
2:B:284:VAL:HG21	2:B:338:SER:C	2.40	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:49:LYS:HG3	1:A:67:ILE:HD13	1.96	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: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
1:A:50:MET:HE2	1:A:58:ILE:HG21	1.97	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:53:ASP:CG	1:A:54:SER:N	2.74	0.46
1:A:91:ALA:HA	1:A:96:THR:OG1	2.15	0.46
1:A:183:ALA:CB	1:A:192:VAL:HG12	2.45	0.46
2:B:240:LEU:O	2:B:319:MET:HE2	2.16	0.46
1:A:163:ASN:ND2	2:B:127:ARG:HH22	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:479:ASP:C	1:A:481:ASN:N	2.74	0.45
2:B:219:VAL:HG21	2:B:322:LEU:HD11	1.98	0.45
2:B:402:ASP:OD2	2:B:497:ARG:HB2	2.17	0.45
1:A:122:VAL:HG21	1:A:429:ARG:HB3	1.98	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:153:LYS:HE3	1:A:490:GLY:CA	2.47	0.45
1:A:486:MET:HB3	1:A:491:VAL:CG2	2.45	0.45
1:A:207:VAL:C	1:A:209:ASP:H	2.24	0.44
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
1:A:206:SER:HB3	1:A:209:ASP:CG	2.43	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
2:B:188:ASP:C	2:B:190:LYS:N	2.74	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
2:B:85:LYS:C	2:B:87:GLN:N	2.75	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:359:PHE:HD2	1:A:361:MET:HE3	1.83	0.43
1:A:417:MET:SD	1:A:468:GLU:HG3	2.58	0.43
1:A:455:ASP:OD2	1:A:458:ASN:HB2	2.18	0.43
1:A:57:ASP:HB3	1:A:58:ILE:H	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:THR:O	2:B:86:THR:CG2	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:128:ARG:HH22	1:A:503:GLU:CD	2.26	0.42
1:A:17:ARG:HH21	1:A:19:GLN:HG3	1.84	0.42
1:A:174:LEU:HD22	1:A:212:PHE:HB2	2.01	0.42
1:A:297:VAL:O	1:A:300:HIS:HB3	2.19	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
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
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:HH11	2:B:44:ARG:HG2	1.85	0.41
2:B:89:SER:HB3	2:B:91:VAL:HG23	2.02	0.41
1:A:102:LEU:HD12	1:A:102:LEU:HA	1.91	0.41
2:B:67:LEU:HD12	2:B:67:LEU:HA	1.91	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
1:A:417:MET:HE2	1:A:417:MET:HB3	1.81	0.41
2:B:478:ASN:O	2:B:482:GLY:N	2.49	0.41
2:B:484:ILE:HD12	2:B:484:ILE:N	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:48:LYS:O	2:B:59:ILE:HA	2.20	0.41
2:B:292:GLN:HE21	2:B:319:MET:HG2	1.86	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
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:125:GLY:HA3	2:B:434:ALA:HB3	2.02	0.41
2:B:224:VAL:HG12	2:B:228:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:ILE:HG21	2:B:263:ILE:HG13	2.03	0.41
1:A:351:LYS:HE2	1:A:351:LYS:HB3	1.77	0.41
1:A:485:ASP:OD2	1:A:487:LYS:HB3	2.21	0.41
2:B:347:ARG:HH11	2:B:347:ARG:HB2	1.85	0.40
1:A:68:LEU:HB2	1:A:85:SER:OG	2.21	0.40
1:A:485:ASP:CG	1:A:487:LYS:HB3	2.46	0.40
1:A:485:ASP:OD1	1:A:487:LYS:HB3	2.22	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:442:GLU:C	1:A:445:PRO:HD2	2.46	0.40
1:A:196:ASN:HD22	1:A:196:ASN:HA	1.75	0.40
2:B:36:SER:O	2:B:48:LYS:HE3	2.21	0.40
2:B:485:GLU:OE1	2:B:490:ASN:OD1	2.39	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%)	7	16
2	B	500/543 (92%)	477 (95%)	18 (4%)	5 (1%)	12	28
All	All	1001/1088 (92%)	941 (94%)	47 (5%)	13 (1%)	9	21

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

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Mol	Chain	Res	Type
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%)	377 (92%)	34 (8%)	10	23
2	B	410/446 (92%)	356 (87%)	54 (13%)	4	8
All	All	821/888 (92%)	733 (89%)	88 (11%)	6	14

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	57	ASP
1	A	92	VAL
1	A	122	VAL
1	A	136	LYS
1	A	139	ASP
1	A	146	THR
1	A	156	LEU
1	A	166	LEU
1	A	184	GLU
1	A	189	LYS
1	A	194	THR
1	A	229	ASP
1	A	230	VAL

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Mol	Chain	Res	Type
1	A	240	ASP
1	A	243	LEU
1	A	249	GLU
1	A	251	GLU
1	A	266	LEU
1	A	316	SER
1	A	333	LEU
1	A	337	THR
1	A	351	LYS
1	A	354	ASP
1	A	377	THR
1	A	379	HIS
1	A	381	VAL
1	A	388	LEU
1	A	443	ILE
1	A	458	ASN
1	A	467	ASP
1	A	478	LEU
1	A	496	ARG
1	A	518	VAL
2	B	24	LYS
2	B	37	VAL
2	B	49	MET
2	B	51	VAL
2	B	54	LEU
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	203	LYS
2	B	209	ASP
2	B	232	VAL
2	B	239	LEU

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Mol	Chain	Res	Type
2	B	248	LYS
2	B	250	GLU
2	B	305	ARG
2	B	311	VAL
2	B	340	SER
2	B	347	ARG
2	B	351	VAL
2	B	352	LYS
2	B	359	THR
2	B	361	VAL
2	B	362	THR
2	B	366	ASN
2	B	370	VAL
2	B	386	GLU
2	B	391	ASP
2	B	396	VAL
2	B	419	ARG
2	B	421	ARG
2	B	425	GLN
2	B	461	LEU
2	B	462	LEU
2	B	488	VAL
2	B	489	LYS
2	B	490	ASN
2	B	492	VAL
2	B	496	ILE
2	B	503	ILE
2	B	504	GLU
2	B	507	THR
2	B	514	LEU
2	B	519	VAL
2	B	520	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) 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

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Mol	Chain	Res	Type
1	A	196	ASN
1	A	233	ASN
1	A	267	ASN
1	A	299	GLN
1	A	365	ASN
1	A	389	ASN
1	A	424	ASN
1	A	431	GLN
1	A	451	ASN
1	A	480	ASN
2	B	26	ASN
2	B	35	ASN
2	B	115	GLN
2	B	118	HIS
2	B	161	ASN
2	B	197	ASN
2	B	204	GLN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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 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.