



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:05 PM UTC

PDB ID : 3P26 / pdb_00003p26
Title : Crystal structure of *S. cerevisiae* Hbs1 protein (apo-form), a translational GTPase involved in RNA quality control pathways and interacting with Dom34/Pelota
Authors : van den Elzen, A.; Henri, J.; Lazar, N.; Gas, M.E.; Durand, D.; Lacroute, F.; Nicaise, M.; van Tilbeurgh, H.; Sraphin, B.; Graille, M.; Paris-Sud Yeast Structural Genomics (YSG)
Deposited on : 2010-10-01
Resolution : 2.50 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

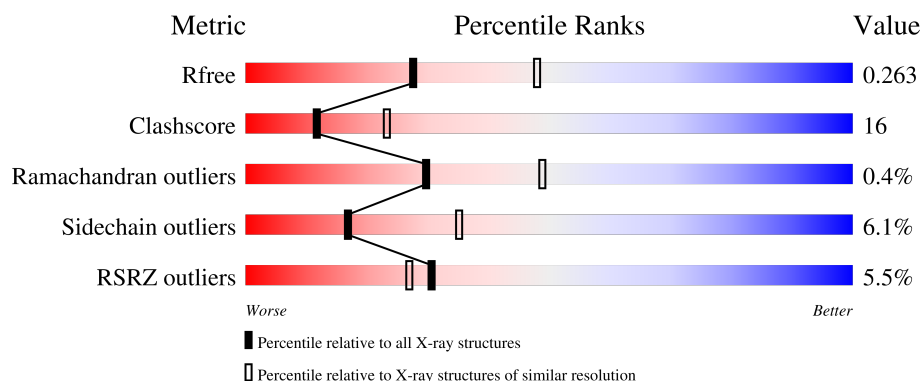
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	483	5% 61% 27% • 10%
1	B	483	5% 58% 28% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7161 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 Elongation factor 1 alpha-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3429	2182	591	643	13			
1	B	439	Total	C	N	O	S	0	0	0
			3457	2199	597	648	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	612	HIS	-	expression tag	UNP P32769
A	613	HIS	-	expression tag	UNP P32769
A	614	HIS	-	expression tag	UNP P32769
A	615	HIS	-	expression tag	UNP P32769
A	616	HIS	-	expression tag	UNP P32769
A	617	HIS	-	expression tag	UNP P32769
B	612	HIS	-	expression tag	UNP P32769
B	613	HIS	-	expression tag	UNP P32769
B	614	HIS	-	expression tag	UNP P32769
B	615	HIS	-	expression tag	UNP P32769
B	616	HIS	-	expression tag	UNP P32769
B	617	HIS	-	expression tag	UNP P32769

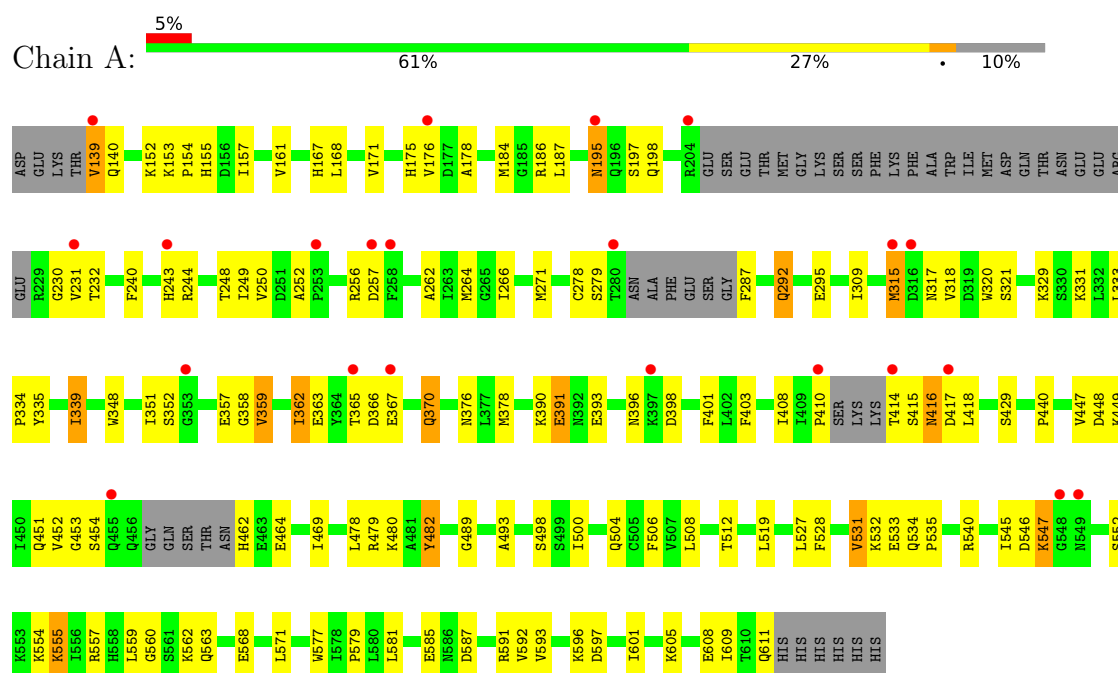
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	135	Total	O	0	0
			135	135		
2	B	140	Total	O	0	0
			140	140		

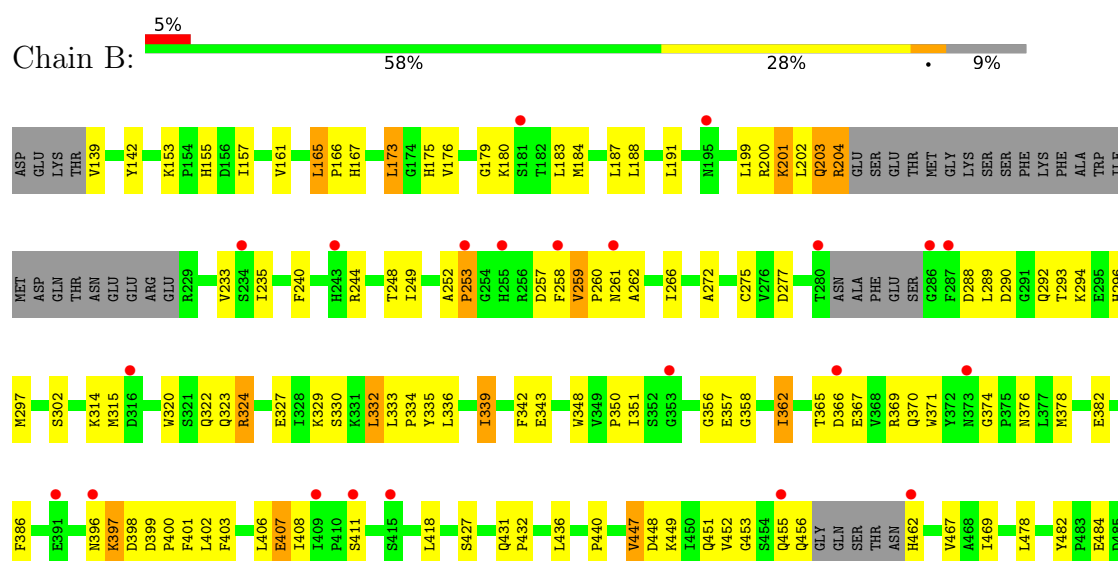
3 Residue-property plots

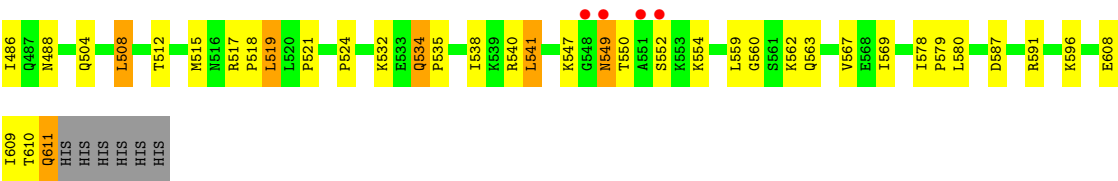
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Elongation factor 1 alpha-like protein



• Molecule 1: Elongation factor 1 alpha-like protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	110.63Å 110.63Å 188.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.09 – 2.50 34.09 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.7 (34.09-2.50) 95.7 (34.09-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.35 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.216 , 0.271 0.209 , 0.263	Depositor DCC
R_{free} test set	1974 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7161	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.9764e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.42	0/3493	0.80	3/4719 (0.1%)
1	B	0.41	0/3522	0.81	6/4757 (0.1%)
All	All	0.42	0/7015	0.81	9/9476 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	482	TYR	CA-C-N	7.51	127.54	119.28
1	B	482	TYR	C-N-CA	7.51	127.54	119.28
1	B	397	LYS	N-CA-C	-6.23	105.64	113.18
1	B	374	GLY	N-CA-C	5.96	119.44	112.23
1	A	416	ASN	N-CA-C	-5.62	105.37	114.09
1	A	482	TYR	CA-C-N	5.15	124.82	119.56
1	A	482	TYR	C-N-CA	5.15	124.82	119.56
1	B	374	GLY	CA-C-N	5.08	125.01	119.78
1	B	374	GLY	C-N-CA	5.08	125.01	119.78

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	3429	0	3463	112	0
1	B	3457	0	3498	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	135	0	0	4	0
2	B	140	0	0	4	0
All	All	7161	0	6961	220	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 (220) 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:512:THR:HG22	1:A:563:GLN:H	1.12	1.12
1:B:512:THR:HG22	1:B:563:GLN:H	1.12	1.07
1:A:608:GLU:HG3	1:B:608:GLU:HG3	1.48	0.95
1:A:512:THR:CG2	1:A:563:GLN:H	1.79	0.94
1:B:240:PHE:HE1	1:B:249:ILE:HD11	1.37	0.89
1:B:365:THR:HG22	1:B:367:GLU:H	1.37	0.88
1:A:195:ASN:HD22	1:A:197:SER:H	1.21	0.86
1:A:243:HIS:CD2	1:A:244:ARG:HG3	2.12	0.84
1:A:512:THR:HG22	1:A:563:GLN:N	1.94	0.80
1:A:547:LYS:HA	1:A:547:LYS:HE2	1.62	0.80
1:A:365:THR:HG22	1:A:367:GLU:H	1.46	0.79
1:B:396:ASN:HB3	1:B:398:ASP:H	1.49	0.76
1:A:287:PHE:O	1:A:331:LYS:HD3	1.86	0.75
1:A:318:VAL:HG12	1:A:321:SER:HB3	1.68	0.75
1:B:512:THR:HG21	1:B:560:GLY:O	1.87	0.75
1:A:195:ASN:HB2	1:A:198:GLN:OE1	1.87	0.75
1:B:259:VAL:HB	1:B:260:PRO:HD3	1.70	0.73
1:B:512:THR:CG2	1:B:563:GLN:H	1.95	0.73
1:B:452:VAL:HG22	1:B:453:GLY:H	1.55	0.72
1:B:175:HIS:CE1	1:B:176:VAL:HG22	2.24	0.72
1:B:199:LEU:O	1:B:203:GLN:HG2	1.89	0.72
1:B:235:ILE:HD11	1:B:406:LEU:HD13	1.71	0.71
1:B:153:LYS:O	1:B:155:HIS:HD2	1.72	0.71
1:A:512:THR:HG21	1:A:560:GLY:O	1.90	0.71
1:B:357:GLU:HA	1:B:362:ILE:HG13	1.72	0.70
1:B:252:ALA:HB1	1:B:253:PRO:HD2	1.73	0.70
1:A:528:PHE:HB2	1:A:593:VAL:HG22	1.74	0.70
1:B:512:THR:HG22	1:B:563:GLN:N	1.97	0.70
1:B:200:ARG:HA	1:B:203:GLN:HG3	1.75	0.69
1:A:555:LYS:HG2	1:A:557:ARG:NH2	2.08	0.68
1:A:418:LEU:HD11	1:A:479:ARG:HG3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:ILE:HG22	1:A:611:GLN:H	1.59	0.67
1:A:187:LEU:HD11	1:A:378:MET:HE2	1.76	0.67
1:B:233:VAL:HG22	1:B:407:GLU:OE2	1.93	0.66
1:B:367:GLU:O	1:B:370:GLN:HG2	1.95	0.66
1:B:515:MET:HE1	1:B:519:LEU:HD22	1.77	0.66
1:A:555:LYS:HG2	1:A:557:ARG:CZ	2.27	0.65
1:B:258:PHE:CZ	1:B:292:GLN:HB2	2.32	0.65
1:B:183:LEU:HD13	1:B:351:ILE:HD12	1.78	0.64
1:A:271:MET:HE1	1:A:309:ILE:HG13	1.78	0.64
1:A:396:ASN:HB3	1:A:398:ASP:H	1.61	0.64
1:B:336:LEU:O	1:B:339:ILE:HG22	1.97	0.64
1:A:292:GLN:O	1:A:295:GLU:HB3	1.99	0.63
1:A:452:VAL:HG22	1:A:453:GLY:H	1.64	0.63
1:B:532:LYS:HD2	1:B:578:ILE:HD12	1.79	0.63
1:B:508:LEU:HD22	1:B:569:ILE:CG1	2.29	0.62
1:B:315:MET:HE3	1:B:320:TRP:HA	1.82	0.61
1:A:167:HIS:HE1	1:A:248:THR:OG1	1.83	0.61
1:A:417:ASP:HB2	1:A:480:LYS:HA	1.84	0.60
1:A:504:GLN:HG2	1:A:577:TRP:HH2	1.66	0.60
1:A:547:LYS:HA	1:A:547:LYS:CE	2.32	0.60
1:B:362:ILE:HG13	1:B:362:ILE:O	2.00	0.60
1:A:414:THR:N	1:A:415:SER:HG	2.00	0.60
1:B:187:LEU:HD11	1:B:378:MET:HE2	1.84	0.59
1:B:431:GLN:HG2	1:B:467:VAL:HG22	1.85	0.59
1:A:462:HIS:CG	1:A:462:HIS:O	2.55	0.59
1:B:452:VAL:HG22	1:B:453:GLY:N	2.18	0.59
1:A:390:LYS:O	1:A:393:GLU:HG2	2.04	0.58
1:B:448:ASP:O	1:B:449:LYS:HG2	2.03	0.58
1:B:244:ARG:HD3	1:B:382:GLU:OE2	2.04	0.58
1:A:279:SER:HB3	1:A:317:ASN:HB2	1.86	0.57
1:B:175:HIS:HB2	1:B:290:ASP:OD2	2.05	0.57
1:A:358:GLY:O	1:A:376:ASN:HB2	2.05	0.57
1:B:609:ILE:HG22	1:B:611:GLN:H	1.68	0.57
1:A:563:GLN:HB3	2:A:680:HOH:O	2.04	0.57
1:B:166:PRO:HG2	1:B:386:PHE:CE1	2.40	0.56
1:B:508:LEU:HD22	1:B:569:ILE:HG12	1.87	0.56
1:A:452:VAL:HG22	1:A:453:GLY:N	2.20	0.56
1:A:362:ILE:O	1:A:362:ILE:HG13	2.06	0.56
1:A:414:THR:N	1:A:415:SER:HA	2.20	0.56
1:A:504:GLN:HG2	1:A:577:TRP:CH2	2.40	0.56
1:A:489:GLY:HA3	1:A:532:LYS:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:GLN:NE2	1:A:535:PRO:HD2	2.21	0.55
1:B:521:PRO:HD3	1:B:541:LEU:HD22	1.88	0.55
1:B:293:THR:O	1:B:297:MET:HG2	2.07	0.55
1:B:358:GLY:O	1:B:376:ASN:HB2	2.06	0.55
1:B:288:ASP:HA	2:B:659:HOH:O	2.07	0.55
1:A:440:PRO:HD3	1:A:579:PRO:HD3	1.89	0.54
1:A:552:SER:OG	1:A:554:LYS:HE3	2.07	0.54
1:B:187:LEU:HD11	1:B:378:MET:CE	2.37	0.54
1:B:275:CYS:HB3	2:B:681:HOH:O	2.06	0.54
1:B:322:GLN:HG3	1:B:371:TRP:CE3	2.42	0.54
1:A:171:VAL:HG21	1:A:252:ALA:HB2	1.89	0.54
1:A:231:VAL:HG22	2:A:658:HOH:O	2.06	0.54
1:A:243:HIS:HD2	1:A:244:ARG:HG3	1.64	0.54
1:A:609:ILE:C	1:A:611:GLN:H	2.14	0.54
1:A:512:THR:HG23	1:A:562:LYS:N	2.23	0.54
1:B:609:ILE:HG22	1:B:611:GLN:N	2.23	0.54
1:B:157:ILE:O	1:B:161:VAL:HG23	2.08	0.54
1:A:195:ASN:HB3	1:A:198:GLN:H	1.74	0.53
1:A:157:ILE:HD13	1:A:429:SER:OG	2.09	0.53
1:B:333:LEU:HB3	1:B:334:PRO:HD3	1.91	0.53
1:A:184:MET:HA	1:A:184:MET:HE2	1.91	0.52
1:B:252:ALA:HB3	1:B:261:ASN:OD1	2.10	0.52
1:B:532:LYS:HE2	2:B:643:HOH:O	2.08	0.52
1:A:596:LYS:HG2	1:A:601:ILE:HD13	1.91	0.51
1:A:448:ASP:O	1:A:449:LYS:HG3	2.10	0.51
1:A:357:GLU:HA	1:A:362:ILE:HG13	1.92	0.51
1:B:202:LEU:C	1:B:204:ARG:H	2.17	0.51
1:B:277:ASP:OD1	1:B:314:LYS:HD2	2.11	0.51
1:B:451:GLN:HE21	1:B:456:GLN:HA	1.76	0.51
1:B:418:LEU:HA	1:B:478:LEU:O	2.11	0.51
1:B:157:ILE:HG12	1:B:397:LYS:HE3	1.93	0.51
1:A:418:LEU:CD1	1:A:479:ARG:HG3	2.41	0.51
1:B:289:LEU:HG	1:B:294:LYS:HG3	1.92	0.51
1:B:366:ASP:HA	1:B:369:ARG:HB2	1.92	0.51
1:A:153:LYS:O	1:A:154:PRO:C	2.55	0.50
1:B:235:ILE:CD1	1:B:406:LEU:HD13	2.42	0.50
1:A:333:LEU:HB3	1:A:334:PRO:HD3	1.92	0.50
1:A:506:PHE:HE1	1:A:508:LEU:HD21	1.77	0.49
1:B:258:PHE:CZ	1:B:296:HIS:CE1	3.00	0.49
1:A:365:THR:HG22	1:A:366:ASP:N	2.26	0.49
1:B:302:SER:O	1:B:591:ARG:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:THR:OG1	1:A:415:SER:HA	2.13	0.49
1:A:335:TYR:CZ	1:A:339:ILE:HD12	2.48	0.48
1:B:332:LEU:HD13	1:B:336:LEU:HG	1.95	0.48
1:B:524:PRO:O	1:B:596:LYS:HE3	2.14	0.48
1:A:187:LEU:HD11	1:A:378:MET:CE	2.43	0.48
1:B:329:LYS:HE3	1:B:348:TRP:CE2	2.48	0.48
1:B:402:LEU:HB2	1:B:427:SER:HB3	1.96	0.48
1:B:508:LEU:HD22	1:B:569:ILE:HG13	1.95	0.48
1:B:173:LEU:HD22	1:B:272:ALA:HB1	1.96	0.48
1:A:418:LEU:HA	1:A:478:LEU:O	2.14	0.48
1:A:240:PHE:CE1	1:A:249:ILE:HD11	2.48	0.47
1:A:367:GLU:O	1:A:370:GLN:HG2	2.14	0.47
1:A:401:PHE:CZ	1:A:403:PHE:HB2	2.49	0.47
1:B:335:TYR:CZ	1:B:339:ILE:HD12	2.49	0.47
1:B:440:PRO:HG3	1:B:579:PRO:HD3	1.96	0.47
1:B:153:LYS:O	1:B:155:HIS:CD2	2.62	0.47
1:B:323:GLN:HG2	2:B:677:HOH:O	2.14	0.47
1:B:320:TRP:HZ3	1:B:350:PRO:HB2	1.80	0.47
1:A:157:ILE:O	1:A:161:VAL:HG23	2.14	0.47
1:A:231:VAL:HG13	1:A:408:ILE:O	2.15	0.47
1:A:318:VAL:HG12	1:A:318:VAL:O	2.15	0.47
1:A:362:ILE:HG23	2:A:637:HOH:O	2.14	0.47
1:B:183:LEU:HD23	1:B:275:CYS:SG	2.54	0.47
1:A:528:PHE:HB2	1:A:593:VAL:CG2	2.45	0.47
1:A:365:THR:HG22	1:A:367:GLU:N	2.23	0.47
1:B:320:TRP:CZ3	1:B:350:PRO:HB2	2.50	0.47
1:B:139:VAL:HG11	1:B:142:TYR:CE2	2.50	0.47
1:B:436:LEU:HD12	1:B:436:LEU:C	2.41	0.46
1:A:391:GLU:H	1:A:391:GLU:HG2	1.41	0.46
1:A:527:LEU:HD11	1:A:592:VAL:HB	1.98	0.46
1:B:538:ILE:HD12	1:B:567:VAL:HG11	1.97	0.46
1:B:327:GLU:O	1:B:330:SER:OG	2.33	0.46
1:A:329:LYS:HE3	1:A:348:TRP:NE1	2.30	0.46
1:B:258:PHE:CZ	1:B:296:HIS:CD2	3.04	0.46
1:A:231:VAL:HG23	1:A:232:THR:N	2.31	0.46
1:A:256:ARG:H	1:A:256:ARG:HG3	1.49	0.46
1:A:609:ILE:CG2	1:A:611:GLN:H	2.25	0.46
1:B:257:ASP:O	1:B:258:PHE:C	2.59	0.46
1:B:512:THR:HG23	1:B:562:LYS:N	2.31	0.46
1:A:315:MET:HE2	1:A:315:MET:HA	1.98	0.45
1:A:167:HIS:CE1	1:A:248:THR:OG1	2.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:MET:HE2	1:A:531:VAL:O	2.16	0.45
1:A:416:ASN:HB3	1:A:418:LEU:HD13	1.97	0.45
1:B:188:LEU:HA	1:B:191:LEU:HD12	1.99	0.45
1:A:333:LEU:HD12	1:A:333:LEU:O	2.17	0.45
1:A:546:ASP:O	1:A:547:LYS:HE2	2.17	0.44
1:A:552:SER:OG	1:A:554:LYS:CE	2.65	0.44
1:B:342:PHE:O	1:B:343:GLU:C	2.60	0.44
1:B:365:THR:HG22	1:B:366:ASP:N	2.33	0.44
1:B:455:GLN:OE1	1:B:462:HIS:N	2.51	0.44
1:B:184:MET:HE2	1:B:184:MET:HA	2.00	0.44
1:B:262:ALA:O	1:B:266:ILE:HG13	2.17	0.44
1:B:176:VAL:HG13	1:B:292:GLN:OE1	2.18	0.44
1:B:240:PHE:CE1	1:B:249:ILE:HD11	2.30	0.44
1:B:517:ARG:HA	1:B:518:PRO:HD3	1.89	0.44
1:B:356:GLY:O	1:B:362:ILE:HG23	2.17	0.44
1:B:401:PHE:CZ	1:B:403:PHE:HB2	2.53	0.44
1:A:171:VAL:HG21	1:A:252:ALA:CB	2.48	0.43
1:B:519:LEU:HB2	1:B:559:LEU:HB3	2.00	0.43
1:B:432:PRO:HA	1:B:447:VAL:HG22	2.01	0.43
1:A:231:VAL:HG23	1:A:232:THR:H	1.84	0.43
1:A:365:THR:CG2	1:A:366:ASP:N	2.81	0.43
1:A:401:PHE:O	1:A:493:ALA:HA	2.19	0.43
1:A:587:ASP:O	1:A:591:ARG:HG2	2.17	0.43
1:B:167:HIS:HE1	1:B:248:THR:OG1	2.00	0.43
1:B:408:ILE:HD11	1:B:486:ILE:HG22	2.00	0.43
1:A:139:VAL:O	1:A:140:GLN:C	2.62	0.43
1:A:318:VAL:CG1	1:A:321:SER:HB3	2.45	0.43
1:B:179:GLY:O	1:B:180:LYS:C	2.62	0.43
1:A:175:HIS:ND1	1:A:176:VAL:N	2.67	0.43
1:B:258:PHE:CZ	1:B:296:HIS:NE2	2.87	0.42
1:B:488:ASN:O	1:B:532:LYS:HE3	2.19	0.42
1:A:175:HIS:O	1:A:178:ALA:HB3	2.19	0.42
1:B:165:LEU:HD12	1:B:165:LEU:HA	1.88	0.42
1:B:534:GLN:NE2	1:B:535:PRO:HD2	2.33	0.42
1:B:587:ASP:O	1:B:591:ARG:HG2	2.19	0.42
1:A:231:VAL:HG12	1:A:410:PRO:HG3	2.01	0.42
1:A:168:LEU:HD11	1:A:271:MET:HG2	2.01	0.42
1:B:201:LYS:HE3	1:B:201:LYS:HA	2.00	0.42
1:A:320:TRP:HZ2	1:A:352:SER:HB2	1.84	0.42
1:A:605:LYS:NZ	1:B:549:ASN:HB3	2.35	0.42
1:B:552:SER:OG	1:B:554:LYS:HE3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ARG:HG3	1:A:359:VAL:HG11	2.01	0.42
1:B:547:LYS:HD3	1:B:547:LYS:HA	1.50	0.42
1:B:166:PRO:HG2	1:B:386:PHE:CZ	2.54	0.41
1:B:294:LYS:HG2	1:B:335:TYR:CZ	2.54	0.41
1:A:240:PHE:HE1	1:A:249:ILE:HD11	1.84	0.41
1:A:500:ILE:HG12	1:A:581:LEU:HD13	2.01	0.41
1:A:540:ARG:HD3	1:A:568:GLU:OE2	2.20	0.41
1:A:262:ALA:O	1:A:266:ILE:HG13	2.20	0.41
1:A:153:LYS:O	1:A:155:HIS:HD2	2.03	0.41
1:A:498:SER:HA	2:A:39:HOH:O	2.20	0.41
1:A:278:CYS:CB	1:A:315:MET:HE3	2.51	0.41
1:B:200:ARG:HA	1:B:203:GLN:CG	2.48	0.41
1:B:365:THR:HG22	1:B:367:GLU:N	2.20	0.41
1:A:449:LYS:HE2	1:A:464:GLU:OE2	2.20	0.41
1:A:512:THR:HG22	1:A:563:GLN:O	2.21	0.41
1:A:519:LEU:HB2	1:A:559:LEU:HB3	2.02	0.41
1:B:257:ASP:O	1:B:261:ASN:HB3	2.21	0.41
1:B:324:ARG:O	1:B:327:GLU:HG2	2.21	0.41
1:B:399:ASP:HA	1:B:400:PRO:HD3	1.92	0.41
1:A:152:LYS:NZ	1:A:448:ASP:HB2	2.36	0.40
1:A:585:GLU:CD	1:B:540:ARG:HH22	2.29	0.40
1:A:195:ASN:CB	1:A:198:GLN:HG3	2.51	0.40
1:A:367:GLU:O	1:A:370:GLN:CG	2.70	0.40
1:A:230:GLY:HA2	1:A:410:PRO:HD3	2.02	0.40
1:A:482:TYR:N	1:A:482:TYR:CD1	2.89	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	425/483 (88%)	415 (98%)	9 (2%)	1 (0%)	43 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	431/483 (89%)	405 (94%)	24 (6%)	2 (0%)	24	43
All	All	856/966 (89%)	820 (96%)	33 (4%)	3 (0%)	30	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	203	GLN
1	B	253	PRO
1	A	359	VAL

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	384/427 (90%)	361 (94%)	23 (6%)	17	36
1	B	387/427 (91%)	363 (94%)	24 (6%)	16	34
All	All	771/854 (90%)	724 (94%)	47 (6%)	17	35

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	VAL
1	A	195	ASN
1	A	250	VAL
1	A	257	ASP
1	A	292	GLN
1	A	315	MET
1	A	339	ILE
1	A	351	ILE
1	A	362	ILE
1	A	363	GLU
1	A	370	GLN
1	A	391	GLU
1	A	447	VAL

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Mol	Chain	Res	Type
1	A	451	GLN
1	A	454	SER
1	A	469	ILE
1	A	531	VAL
1	A	533	GLU
1	A	545	ILE
1	A	547	LYS
1	A	555	LYS
1	A	571	LEU
1	A	597	ASP
1	B	165	LEU
1	B	173	LEU
1	B	201	LYS
1	B	204	ARG
1	B	259	VAL
1	B	324	ARG
1	B	332	LEU
1	B	339	ILE
1	B	362	ILE
1	B	407	GLU
1	B	411	SER
1	B	447	VAL
1	B	469	ILE
1	B	484	GLU
1	B	504	GLN
1	B	508	LEU
1	B	519	LEU
1	B	534	GLN
1	B	541	LEU
1	B	549	ASN
1	B	550	THR
1	B	580	LEU
1	B	610	THR
1	B	611	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	HIS
1	A	167	HIS
1	A	195	ASN
1	A	261	ASN

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Mol	Chain	Res	Type
1	A	307	ASN
1	A	323	GLN
1	A	345	ASN
1	A	347	ASN
1	A	392	ASN
1	A	456	GLN
1	A	487	GLN
1	A	611	GLN
1	B	155	HIS
1	B	167	HIS
1	B	268	GLN
1	B	307	ASN
1	B	345	ASN
1	B	383	ASN
1	B	392	ASN
1	B	451	GLN
1	B	456	GLN
1	B	488	ASN
1	B	534	GLN

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

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, 95th 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	435/483 (90%)	0.23	22 (5%) 33 29	24, 42, 72, 99	0
1	B	439/483 (90%)	0.24	26 (5%) 28 24	24, 43, 72, 104	0
All	All	874/966 (90%)	0.24	48 (5%) 30 27	24, 42, 72, 104	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	353	GLY	4.0
1	B	548	GLY	3.9
1	A	548	GLY	3.8
1	A	243	HIS	3.8
1	A	455	GLN	3.7
1	B	396	ASN	3.3
1	B	253	PRO	3.2
1	B	549	ASN	3.1
1	B	353	GLY	2.9
1	B	455	GLN	2.9
1	B	286	GLY	2.8
1	B	316	ASP	2.8
1	B	258	PHE	2.8
1	A	397	LYS	2.7
1	A	414	THR	2.7
1	A	204	ARG	2.6
1	A	258	PHE	2.6
1	B	373	ASN	2.5
1	B	234	SER	2.5
1	B	280	THR	2.5
1	A	417	ASP	2.4
1	B	255	HIS	2.4
1	B	462	HIS	2.4
1	A	365	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	316	ASP	2.4
1	B	195	ASN	2.4
1	B	411	SER	2.3
1	A	280	THR	2.3
1	A	231	VAL	2.3
1	B	181	SER	2.3
1	A	139	VAL	2.3
1	A	549	ASN	2.2
1	B	415	SER	2.2
1	B	287	PHE	2.2
1	B	551	ALA	2.2
1	B	243	HIS	2.2
1	A	315	MET	2.2
1	A	367	GLU	2.2
1	A	253	PRO	2.1
1	B	409	ILE	2.1
1	A	257	ASP	2.1
1	A	176	VAL	2.1
1	B	261	ASN	2.1
1	B	391	GLU	2.1
1	B	366	ASP	2.1
1	A	410	PRO	2.1
1	A	195	ASN	2.0
1	B	552	SER	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.