Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 07:44 AM EST

PDB ID	:	3P26
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 (i) 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 (i)) were used in the production of this report:

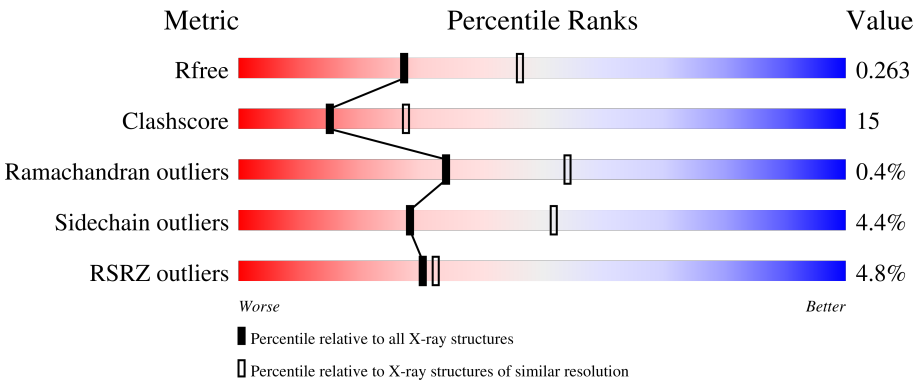
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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% 63% 26% • 10%
1	B	483	4% 61% 27% • 9%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	435	3429	2182	591	643	13	0	0	0
1	B	439	3457	2199	597	648	13	0	0	0

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.

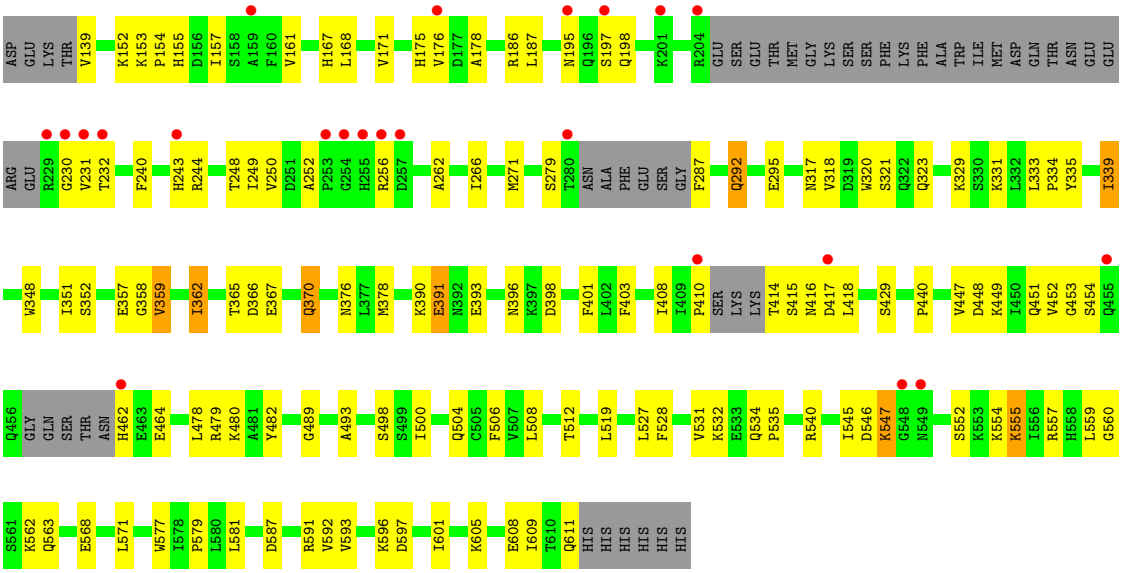
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	135	135	135	0	0
2	B	140	140	140	0	0

3 Residue-property plots (i)

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.

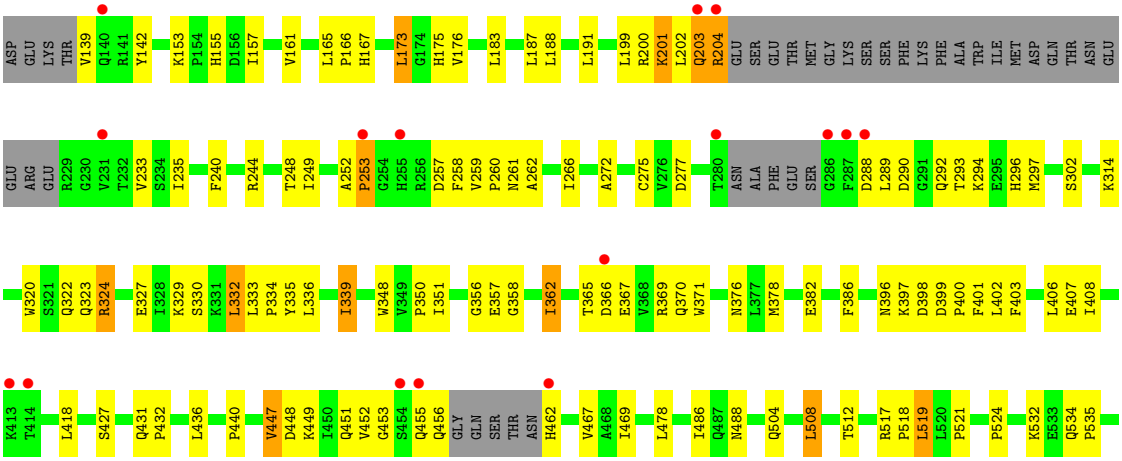
• Molecule 1: Elongation factor 1 alpha-like protein

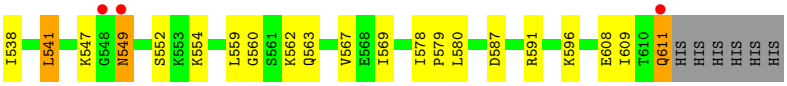
Chain A:



• Molecule 1: Elongation factor 1 alpha-like protein

Chain B:




I538
L541
K547
G548
N549
S552
K553
K554
L559
G560
S561
K562
Q563
V567
E568
I569
I578
P579
L580
D587
R591
K596
E608
I609
T610
Q611
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

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) 95.8 (34.09-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.35 (at 2.51Å)	Xtriage
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 (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	43.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7161	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage'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.*

[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 (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	0.34	0/3493	0.52	0/4719
1	B	0.33	0/3522	0.53	0/4757
All	All	0.34	0/7015	0.53	0/9476

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 (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	105	0
1	B	3457	0	3498	106	0
2	A	135	0	0	4	0
2	B	140	0	0	4	0
All	All	7161	0	6961	209	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 15.

All (209) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:414:THR:N	1:A:415:SER:HG	1.91	0.68
1:A:418:LEU:HD11	1:A:479:ARG:HG3	1.75	0.68
1:A:609:ILE:HG22	1:A:611:GLN:H	1.59	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:431:GLN:HG2	1:B:467:VAL:HG22	1.85	0.59
1:A:462:HIS:O	1:A:462:HIS:CG	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:HG13	1:A:362:ILE:O	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:252:ALA:HB3	1:B:261:ASN:OD1	2.10	0.52
1:B:187:LEU:HD11	1:B:378:MET:HE1	1.92	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: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: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:A:609:ILE:C	1:A:611:GLN:H	2.14	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
1:A:187:LEU:HD11	1:A:378:MET:CE	2.43	0.49
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: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:202:LEU:C	1:B:204:ARG:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:512:THR:HG23	1:B:562:LYS:N	2.31	0.46
1:A:153:LYS:O	1:A:154:PRO:C	2.55	0.45
1:A:167:HIS:CE1	1:A:248:THR:OG1	2.68	0.45
1:A:187:LEU:HD11	1:A:378:MET:HE1	1.98	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:318:VAL:CG1	1:A:321:SER:HB3	2.45	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:436:LEU:HD12	1:B:436:LEU:C	2.41	0.42
1:B:552:SER:OG	1:B:554:LYS:HE3	2.19	0.42
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:B:200:ARG:HA	1:B:203:GLN:CG	2.48	0.41
1:B:257:ASP:O	1:B:258:PHE:C	2.59	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:LEU:HD11	1:B:378:MET:HE2	2.04	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 (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	425/483 (88%)	415 (98%)	9 (2%)	1 (0%)	47	68
1	B	431/483 (89%)	405 (94%)	24 (6%)	2 (0%)	29	48
All	All	856/966 (89%)	820 (96%)	33 (4%)	3 (0%)	34	54

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 (i)

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	384/427 (90%)	366 (95%)	18 (5%)	26	49
1	B	387/427 (91%)	371 (96%)	16 (4%)	30	55
All	All	771/854 (90%)	737 (96%)	34 (4%)	28	52

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	VAL
1	A	250	VAL
1	A	292	GLN
1	A	323	GLN
1	A	339	ILE
1	A	351	ILE
1	A	362	ILE
1	A	370	GLN
1	A	391	GLU
1	A	447	VAL
1	A	451	GLN
1	A	454	SER
1	A	531	VAL
1	A	545	ILE
1	A	547	LYS
1	A	555	LYS
1	A	571	LEU
1	A	597	ASP
1	B	173	LEU
1	B	201	LYS
1	B	204	ARG
1	B	324	ARG
1	B	332	LEU
1	B	339	ILE
1	B	362	ILE
1	B	447	VAL
1	B	469	ILE
1	B	504	GLN
1	B	508	LEU
1	B	519	LEU
1	B	541	LEU
1	B	549	ASN

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Mol	Chain	Res	Type
1	B	580	LEU
1	B	611	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	HIS
1	A	167	HIS
1	A	195	ASN
1	A	268	GLN
1	A	323	GLN
1	A	345	ASN
1	A	392	ASN
1	A	416	ASN
1	A	487	GLN
1	A	534	GLN
1	B	155	HIS
1	B	167	HIS
1	B	239	HIS
1	B	268	GLN
1	B	345	ASN
1	B	383	ASN
1	B	392	ASN
1	B	416	ASN
1	B	451	GLN
1	B	488	ASN
1	B	534	GLN
1	B	611	GLN

5.3.3 RNA (i)

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.18	23 (5%)	26	28	24, 42, 72, 99	0
1	B	439/483 (90%)	0.20	19 (4%)	35	38	24, 43, 72, 104	0
All	All	874/966 (90%)	0.19	42 (4%)	30	32	24, 42, 72, 104	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	462	HIS	5.5
1	B	255	HIS	4.6
1	B	413	LYS	4.4
1	A	229	ARG	4.3
1	A	257	ASP	4.3
1	A	204	ARG	4.2
1	B	231	VAL	4.2
1	A	231	VAL	3.9
1	A	455	GLN	3.6
1	A	254	GLY	3.5
1	A	255	HIS	3.4
1	B	549	ASN	3.4
1	B	455	GLN	3.3
1	B	548	GLY	3.3
1	A	462	HIS	3.2
1	B	204	ARG	3.2
1	B	454	SER	3.1
1	A	548	GLY	3.1
1	B	287	PHE	3.0
1	A	256	ARG	3.0
1	B	288	ASP	3.0
1	A	243	HIS	3.0
1	B	203	GLN	3.0
1	A	232	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	253	PRO	2.7
1	B	286	GLY	2.6
1	A	253	PRO	2.5
1	B	414	THR	2.5
1	A	230	GLY	2.5
1	A	280	THR	2.5
1	A	201	LYS	2.4
1	B	140	GLN	2.4
1	A	410	PRO	2.3
1	A	159	ALA	2.2
1	A	549	ASN	2.2
1	B	611	GLN	2.2
1	A	195	ASN	2.2
1	A	417	ASP	2.1
1	B	280	THR	2.1
1	B	366	ASP	2.1
1	A	176	VAL	2.0
1	A	197	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 monosaccharides 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.