



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:02 AM UTC

PDB ID : 2D4Y / pdb_00002d4y
Title : Crystal structure of a 49K fragment of HAP1 (FlgK)
Authors : Imada, K.; Matsunami, H.; Samatey, A.F.; Nagashima, S.; Namba, K.
Deposited on : 2005-10-25
Resolution : 2.10 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

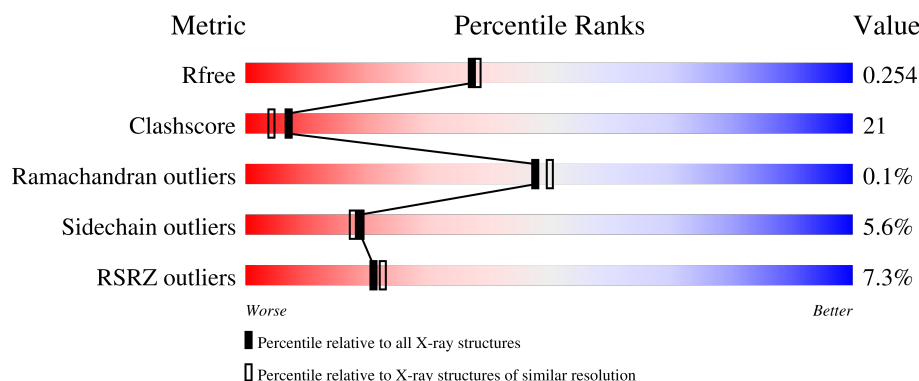
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	463	5% 69% 20% • 7%
1	B	463	8% 66% 23% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7216 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 Flagellar hook-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3236	1987	563	681	5			
1	B	425	Total	C	N	O	S	0	0	0
			3205	1968	558	674	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	MET	-	initiating methionine	UNP P0A1J5
B	64	MET	-	initiating methionine	UNP P0A1J5

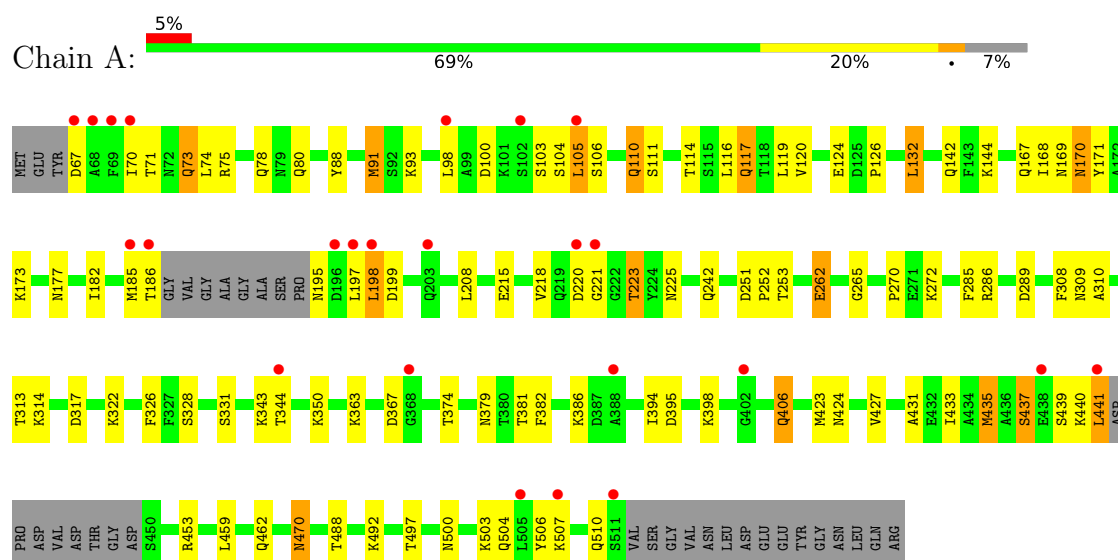
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	395	Total	O	0	0
			395	395		
2	B	380	Total	O	0	0
			380	380		

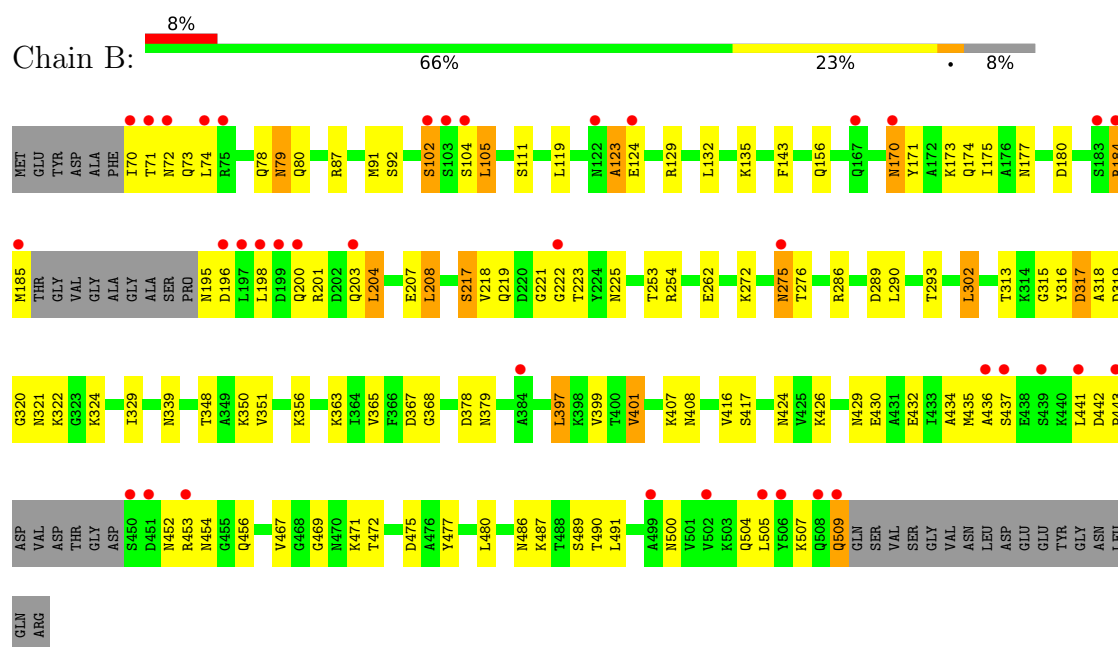
3 Residue-property plots [i](#)

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: Flagellar hook-associated protein 1



• Molecule 1: Flagellar hook-associated protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.93Å 99.70Å 109.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.54 – 2.10 73.76 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.8 (74.54-2.10) 97.8 (73.76-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.219 , 0.255 0.219 , 0.254	Depositor DCC
R_{free} test set	2844 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7216	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.83	2/3266 (0.1%)	1.01	1/4424 (0.0%)
1	B	0.77	0/3235	1.07	7/4383 (0.2%)
All	All	0.80	2/6501 (0.0%)	1.04	8/8807 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	435	MET	SD-CE	-7.17	1.61	1.79
1	A	91	MET	SD-CE	-6.94	1.62	1.79

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	GLY	N-CA-C	-7.59	105.05	114.92
1	B	416	VAL	N-CA-C	7.38	120.28	113.20
1	B	318	ALA	N-CA-C	-6.74	105.06	113.28
1	B	123	ALA	N-CA-C	6.70	120.32	111.75
1	B	368	GLY	N-CA-C	-5.59	107.33	114.37
1	B	102	SER	N-CA-C	-5.46	106.53	114.12
1	B	434	ALA	N-CA-C	5.23	117.62	108.52
1	B	105	LEU	N-CA-C	-5.15	105.84	111.82

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	3236	0	3192	126	0
1	B	3205	0	3165	143	0
2	A	395	0	0	74	3
2	B	380	0	0	93	3
All	All	7216	0	6357	268	4

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 21.

All (268) 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:91:MET:CE	1:A:289:ASP:HB3	1.45	1.43
1:A:91:MET:HE3	1:A:289:ASP:CB	1.60	1.30
1:B:71:THR:HG23	2:B:578:HOH:O	1.32	1.29
1:A:459:LEU:HD23	2:A:832:HOH:O	1.40	1.19
1:A:488:THR:HG23	2:A:720:HOH:O	1.51	1.10
1:B:72:ASN:ND2	2:B:828:HOH:O	1.85	1.10
1:B:489:SER:HB2	2:B:897:HOH:O	1.51	1.10
1:B:276:THR:OG1	2:B:670:HOH:O	1.71	1.07
1:A:88:TYR:O	2:A:835:HOH:O	1.74	1.05
1:B:324:LYS:HD2	2:B:842:HOH:O	1.54	1.04
1:A:343:LYS:HG2	2:A:888:HOH:O	1.56	1.02
1:A:253:THR:OG1	2:A:672:HOH:O	1.77	1.02
1:A:225:ASN:OD1	2:A:834:HOH:O	1.79	0.99
1:B:489:SER:CB	2:B:897:HOH:O	2.10	0.98
1:A:120:VAL:HG12	2:A:867:HOH:O	1.66	0.95
1:B:80:GLN:OE1	2:B:776:HOH:O	1.83	0.95
1:A:503:LYS:NZ	2:A:799:HOH:O	1.76	0.94
1:B:124:GLU:HB3	2:B:737:HOH:O	1.70	0.92
1:B:132:LEU:HD12	2:B:805:HOH:O	1.70	0.91
1:A:91:MET:HE3	1:A:289:ASP:HB3	0.91	0.90
1:B:275:ASN:O	2:B:693:HOH:O	1.92	0.88
1:A:91:MET:HE3	1:A:289:ASP:CG	2.00	0.87
1:B:217:SER:HB2	2:B:546:HOH:O	1.75	0.86
1:B:317:ASP:OD2	2:B:573:HOH:O	1.92	0.86
1:B:275:ASN:HB2	2:B:881:HOH:O	1.75	0.86
1:B:475:ASP:OD1	2:B:762:HOH:O	1.94	0.86
1:A:91:MET:CE	1:A:289:ASP:CB	2.36	0.85
1:B:429:ASN:OD1	2:B:713:HOH:O	1.92	0.85
1:A:100:ASP:HA	2:A:690:HOH:O	1.77	0.84
1:B:424:ASN:ND2	2:B:684:HOH:O	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:GLN:NE2	2:B:622:HOH:O	2.12	0.83
1:B:180:ASP:HB3	2:B:627:HOH:O	1.80	0.80
1:B:276:THR:HG22	2:B:861:HOH:O	1.80	0.79
1:B:456:GLN:HB2	2:B:642:HOH:O	1.82	0.79
1:A:170:ASN:OD1	2:A:627:HOH:O	2.00	0.79
1:A:170:ASN:ND2	2:A:843:HOH:O	2.16	0.79
1:A:117:GLN:NE2	2:A:657:HOH:O	2.15	0.78
1:A:80:GLN:HB3	2:A:775:HOH:O	1.84	0.78
1:A:91:MET:HE1	1:A:289:ASP:HB3	1.63	0.78
1:B:218:VAL:HG23	2:B:650:HOH:O	1.82	0.78
1:A:363:LYS:HD3	2:A:870:HOH:O	1.83	0.77
1:B:272:LYS:NZ	2:B:848:HOH:O	2.17	0.77
1:A:322:LYS:HE3	2:A:891:HOH:O	1.85	0.76
1:B:71:THR:HG21	2:B:729:HOH:O	1.83	0.76
1:B:316:TYR:N	2:B:873:HOH:O	2.10	0.76
1:A:70:ILE:CG2	2:A:624:HOH:O	2.32	0.75
1:B:72:ASN:N	2:B:595:HOH:O	2.12	0.75
1:B:286:ARG:CD	2:B:634:HOH:O	2.34	0.75
1:B:320:GLY:HA2	2:B:706:HOH:O	1.85	0.75
1:B:79:ASN:OD1	1:B:276:THR:HB	1.86	0.75
1:B:201:ARG:NH2	2:B:850:HOH:O	2.18	0.75
1:B:78:GLN:HG3	2:B:885:HOH:O	1.87	0.75
1:A:119:LEU:HG	1:A:435:MET:HE2	1.69	0.75
1:A:272:LYS:HE2	2:A:533:HOH:O	1.85	0.75
1:B:286:ARG:HD3	2:B:634:HOH:O	1.86	0.75
1:B:452:ASN:O	2:B:642:HOH:O	2.05	0.74
1:B:275:ASN:HD22	1:B:275:ASN:H	1.34	0.74
1:A:215:GLU:OE1	2:A:778:HOH:O	2.05	0.74
1:A:225:ASN:CB	2:A:834:HOH:O	2.36	0.73
1:A:185:MET:HG2	2:A:765:HOH:O	1.88	0.73
1:A:195:ASN:N	2:A:889:HOH:O	2.21	0.73
1:A:344:THR:OG1	2:A:848:HOH:O	2.06	0.73
1:B:367:ASP:O	1:B:407:LYS:HG3	1.89	0.72
1:B:70:ILE:HG13	2:B:753:HOH:O	1.88	0.72
1:A:116:LEU:O	1:A:120:VAL:HG23	1.90	0.71
1:A:251:ASP:OD2	2:A:654:HOH:O	2.06	0.71
1:B:426:LYS:HG2	2:B:715:HOH:O	1.90	0.71
1:B:173:LYS:HE2	2:B:673:HOH:O	1.89	0.71
1:B:195:ASN:HB2	2:B:860:HOH:O	1.90	0.71
1:A:105:LEU:HD13	1:A:142:GLN:HG3	1.72	0.70
1:B:174:GLN:HE21	1:B:204:LEU:HD21	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ASP:HB3	1:B:319:ASP:H	1.56	0.69
1:B:417:SER:HB2	2:B:854:HOH:O	1.92	0.69
1:A:286:ARG:HB3	2:A:655:HOH:O	1.92	0.69
1:A:265:GLY:HA2	2:A:903:HOH:O	1.92	0.69
1:A:110:GLN:OE1	1:A:114:THR:OG1	2.11	0.69
1:A:406:GLN:OE1	2:A:732:HOH:O	2.11	0.68
1:A:70:ILE:HG23	2:A:624:HOH:O	1.92	0.68
1:A:124:GLU:HG3	2:A:781:HOH:O	1.93	0.67
1:B:70:ILE:HD12	2:B:646:HOH:O	1.95	0.67
1:B:174:GLN:NE2	1:B:204:LEU:HD21	2.09	0.67
1:B:74:LEU:HD12	2:B:885:HOH:O	1.94	0.67
1:A:195:ASN:OD1	2:A:801:HOH:O	2.12	0.67
1:A:510:GLN:HA	2:A:635:HOH:O	1.95	0.67
1:A:132:LEU:HD12	1:A:433:ILE:HD13	1.77	0.67
1:A:186:THR:O	1:A:186:THR:HG22	1.95	0.65
1:B:316:TYR:O	2:B:873:HOH:O	2.14	0.65
1:A:314:LYS:HE3	2:A:893:HOH:O	1.95	0.65
1:A:406:GLN:HB2	2:A:779:HOH:O	1.96	0.65
1:A:437:SER:OG	1:A:453:ARG:CB	2.44	0.65
1:B:275:ASN:C	2:B:693:HOH:O	2.37	0.64
1:A:91:MET:HB2	2:A:835:HOH:O	1.97	0.64
1:B:184:ARG:CZ	2:B:904:HOH:O	2.45	0.64
1:B:119:LEU:HG	1:B:435:MET:HE2	1.80	0.64
1:B:196:ASP:O	1:B:200:GLN:HG3	1.97	0.64
1:B:436:ALA:N	2:B:873:HOH:O	2.30	0.64
1:B:275:ASN:HD22	1:B:275:ASN:N	1.96	0.64
1:B:500:ASN:HB3	2:B:855:HOH:O	1.97	0.63
1:B:507:LYS:HD3	2:B:851:HOH:O	1.98	0.63
1:A:168:ILE:HG23	1:A:208:LEU:HD11	1.79	0.63
1:A:132:LEU:HD21	2:A:861:HOH:O	1.99	0.63
1:A:350:LYS:HE3	2:A:701:HOH:O	1.97	0.63
1:A:507:LYS:O	1:A:510:GLN:HG2	1.99	0.63
1:B:73:GLN:HG3	2:B:686:HOH:O	1.97	0.62
1:A:225:ASN:CG	2:A:834:HOH:O	2.33	0.62
1:B:171:TYR:O	1:B:175:ILE:HG13	2.00	0.62
1:B:87:ARG:NH2	2:B:741:HOH:O	2.32	0.62
1:B:275:ASN:H	1:B:275:ASN:ND2	1.97	0.61
1:A:117:GLN:HG2	2:A:881:HOH:O	1.99	0.61
1:A:169:ASN:HB3	1:A:242:GLN:NE2	2.16	0.60
1:B:367:ASP:C	1:B:407:LYS:HG3	2.26	0.60
1:B:221:GLY:HA3	2:B:592:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ASN:C	1:B:170:ASN:HD22	2.09	0.60
1:A:437:SER:OG	1:A:453:ARG:HB3	2.01	0.60
1:B:217:SER:HB3	1:B:225:ASN:HB2	1.84	0.60
1:B:221:GLY:CA	2:B:592:HOH:O	2.50	0.60
1:B:104:SER:HB2	2:B:895:HOH:O	2.01	0.60
1:A:398:LYS:HE2	2:A:697:HOH:O	2.03	0.59
1:B:276:THR:CG2	2:B:540:HOH:O	2.50	0.59
1:A:310:ALA:HA	2:A:777:HOH:O	2.02	0.59
1:B:275:ASN:CB	2:B:881:HOH:O	2.40	0.58
1:A:167:GLN:HG2	2:A:597:HOH:O	2.03	0.58
1:A:379:ASN:HB3	2:A:668:HOH:O	2.03	0.58
1:B:443:PRO:HA	2:B:867:HOH:O	2.03	0.58
1:A:437:SER:OG	1:A:453:ARG:HB2	2.04	0.58
1:A:470:ASN:H	1:A:470:ASN:HD22	1.51	0.57
1:B:132:LEU:HA	2:B:805:HOH:O	2.02	0.57
1:B:173:LYS:HB2	2:B:712:HOH:O	2.04	0.57
1:B:477:TYR:OH	2:B:845:HOH:O	2.17	0.57
1:A:91:MET:CB	2:A:835:HOH:O	2.52	0.57
1:B:472:THR:N	2:B:762:HOH:O	2.22	0.57
1:A:386:LYS:CE	2:A:913:HOH:O	2.52	0.57
1:B:286:ARG:HD2	2:B:634:HOH:O	2.03	0.57
1:A:510:GLN:HB3	2:A:719:HOH:O	2.04	0.56
1:B:317:ASP:HB2	1:B:321:ASN:H	1.71	0.56
1:A:394:ILE:O	1:A:395:ASP:C	2.49	0.56
1:A:67:ASP:HA	1:A:70:ILE:HG12	1.86	0.56
1:A:423:MET:O	1:A:424:ASN:ND2	2.39	0.56
1:B:289:ASP:OD1	1:B:487:LYS:NZ	2.33	0.55
1:A:116:LEU:HD13	2:A:861:HOH:O	2.05	0.55
1:B:356:LYS:NZ	2:B:587:HOH:O	2.02	0.55
1:A:262:GLU:OE1	1:A:262:GLU:HA	2.05	0.55
1:B:276:THR:HG23	2:B:693:HOH:O	2.07	0.55
1:B:486:ASN:O	1:B:490:THR:HG23	2.07	0.55
1:A:470:ASN:HD22	1:A:470:ASN:N	2.02	0.55
1:B:104:SER:N	2:B:895:HOH:O	2.39	0.55
1:B:276:THR:HG21	2:B:540:HOH:O	2.05	0.55
1:B:254:ARG:HD3	1:B:286:ARG:CZ	2.37	0.55
1:A:424:ASN:HB2	2:A:798:HOH:O	2.07	0.54
1:B:184:ARG:NE	2:B:904:HOH:O	2.40	0.54
1:A:173:LYS:NZ	2:A:570:HOH:O	2.41	0.54
1:A:223:THR:HB	2:A:789:HOH:O	2.06	0.54
1:B:71:THR:N	2:B:578:HOH:O	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ASN:HB2	2:A:898:HOH:O	2.06	0.54
1:A:309:ASN:O	1:A:313:THR:HG23	2.06	0.54
1:B:272:LYS:O	1:B:272:LYS:HD3	2.08	0.53
1:B:315:GLY:HA3	1:B:454:ASN:ND2	2.23	0.53
1:A:262:GLU:HB3	2:A:711:HOH:O	2.08	0.53
1:A:185:MET:HE1	1:A:197:LEU:HD11	1.91	0.52
1:A:500:ASN:O	1:A:504:GLN:HG3	2.08	0.52
1:B:129:ARG:HD3	1:B:430:GLU:O	2.08	0.52
1:A:367:ASP:OD1	1:A:367:ASP:C	2.53	0.52
1:B:185:MET:C	2:B:859:HOH:O	2.51	0.52
1:B:302:LEU:HD23	1:B:329:ILE:HG12	1.92	0.51
1:A:75:ARG:HD2	2:A:754:HOH:O	2.09	0.51
1:A:177:ASN:OD1	2:A:882:HOH:O	2.19	0.51
1:B:350:LYS:HD3	2:B:725:HOH:O	2.09	0.51
1:B:401:VAL:O	2:B:609:HOH:O	2.19	0.51
1:A:270:PRO:HB2	1:A:272:LYS:HE3	1.92	0.51
1:A:173:LYS:HE3	1:A:242:GLN:NE2	2.25	0.51
1:A:453:ARG:NH1	2:A:896:HOH:O	2.44	0.51
1:A:93:LYS:HE3	2:A:812:HOH:O	2.09	0.50
1:B:207:GLU:OE2	1:B:207:GLU:HA	2.10	0.50
1:B:208:LEU:HD12	1:B:208:LEU:O	2.12	0.50
1:B:452:ASN:HB3	2:B:699:HOH:O	2.11	0.50
1:B:135:LYS:HB2	2:B:805:HOH:O	2.12	0.50
1:A:308:PHE:CE1	2:A:713:HOH:O	2.65	0.50
1:A:492:LYS:HE3	2:A:757:HOH:O	2.11	0.49
1:B:173:LYS:HD2	2:B:791:HOH:O	2.11	0.49
1:A:116:LEU:HB2	2:A:861:HOH:O	2.13	0.49
1:B:253:THR:HB	2:B:858:HOH:O	2.11	0.49
1:B:275:ASN:CG	2:B:693:HOH:O	2.55	0.49
1:A:73:GLN:HE21	1:A:73:GLN:CA	2.24	0.49
1:B:507:LYS:HB3	2:B:851:HOH:O	2.13	0.49
1:A:105:LEU:HD13	1:A:142:GLN:CG	2.40	0.49
1:A:386:LYS:NZ	2:A:913:HOH:O	2.42	0.49
1:B:275:ASN:CA	2:B:881:HOH:O	2.58	0.49
1:B:91:MET:SD	1:B:289:ASP:HB3	2.53	0.49
1:B:437:SER:OG	1:B:453:ARG:HB2	2.13	0.49
1:A:104:SER:HA	2:A:640:HOH:O	2.12	0.48
1:A:67:ASP:HA	1:A:70:ILE:CG1	2.44	0.48
1:A:182:ILE:HD13	1:A:198:LEU:HD12	1.97	0.47
1:A:398:LYS:NZ	2:A:895:HOH:O	2.13	0.47
1:A:386:LYS:HE2	2:A:913:HOH:O	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ASP:CA	1:A:70:ILE:HG12	2.44	0.47
1:A:124:GLU:O	1:A:126:PRO:HD3	2.15	0.47
1:A:453:ARG:NH1	2:A:650:HOH:O	2.37	0.47
1:B:177:ASN:HA	2:B:821:HOH:O	2.13	0.47
1:B:180:ASP:O	1:B:184:ARG:HG2	2.15	0.46
1:A:169:ASN:HB3	1:A:242:GLN:HE22	1.81	0.46
1:A:506:TYR:HD2	2:A:707:HOH:O	1.98	0.46
1:B:184:ARG:HB3	2:B:843:HOH:O	2.16	0.46
1:B:80:GLN:HA	2:B:861:HOH:O	2.15	0.46
1:B:195:ASN:HA	1:B:198:LEU:HD13	1.97	0.46
1:B:348:THR:O	1:B:399:VAL:HG13	2.16	0.46
1:B:219:GLN:HB2	1:B:223:THR:HG22	1.97	0.45
1:A:470:ASN:N	1:A:470:ASN:ND2	2.64	0.45
1:A:326:PHE:HA	1:A:427:VAL:HG23	1.98	0.45
1:A:185:MET:HE1	1:A:197:LEU:CD1	2.47	0.45
1:A:439:SER:C	1:A:441:LEU:N	2.74	0.45
1:B:184:ARG:HD3	2:B:904:HOH:O	2.16	0.45
1:B:71:THR:HG22	2:B:689:HOH:O	2.17	0.45
1:B:471:LYS:HA	2:B:762:HOH:O	2.16	0.45
1:A:91:MET:HE2	1:A:285:PHE:HE1	1.82	0.44
1:B:71:THR:HB	2:B:595:HOH:O	2.17	0.44
1:B:424:ASN:HB2	2:B:568:HOH:O	2.17	0.44
1:B:71:THR:HB	2:B:639:HOH:O	2.18	0.44
1:B:293:THR:HG23	1:B:480:LEU:HD11	2.00	0.44
1:B:472:THR:HG23	2:B:762:HOH:O	2.18	0.44
1:B:184:ARG:HG3	2:B:801:HOH:O	2.18	0.44
1:B:407:LYS:O	1:B:408:ASN:HB2	2.17	0.44
1:B:363:LYS:HB2	2:B:623:HOH:O	2.17	0.43
1:B:173:LYS:HD2	2:B:712:HOH:O	2.18	0.43
1:B:467:VAL:C	1:B:469:GLY:H	2.25	0.43
1:B:507:LYS:CD	2:B:851:HOH:O	2.63	0.43
1:B:222:GLY:O	2:B:727:HOH:O	2.21	0.43
1:A:322:LYS:HG3	2:A:891:HOH:O	2.19	0.43
1:B:79:ASN:ND2	2:B:764:HOH:O	2.52	0.43
1:B:313:THR:O	1:B:322:LYS:HE3	2.19	0.43
1:A:317:ASP:HB2	1:A:431:ALA:O	2.19	0.43
1:A:382:PHE:HA	2:B:713:HOH:O	2.18	0.43
1:B:272:LYS:HD3	1:B:272:LYS:C	2.44	0.42
1:A:70:ILE:HG22	2:A:624:HOH:O	2.10	0.42
1:B:317:ASP:OD1	1:B:432:GLU:HA	2.19	0.42
1:A:91:MET:HE2	1:A:285:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:GLN:HG2	2:B:664:HOH:O	2.20	0.42
1:B:339:ASN:C	2:B:739:HOH:O	2.62	0.42
1:A:424:ASN:ND2	2:A:798:HOH:O	2.51	0.42
1:B:105:LEU:HD21	1:B:143:PHE:CE2	2.55	0.42
1:B:119:LEU:O	1:B:123:ALA:HA	2.20	0.42
1:B:467:VAL:C	1:B:469:GLY:N	2.77	0.42
1:B:505:LEU:HD23	1:B:505:LEU:HA	1.89	0.42
1:A:328:SER:O	1:A:423:MET:HA	2.20	0.42
1:A:167:GLN:HG3	1:A:171:TYR:CE2	2.55	0.41
1:A:199:ASP:CB	2:A:694:HOH:O	2.67	0.41
1:A:199:ASP:HB2	2:A:694:HOH:O	2.20	0.41
1:B:442:ASP:HA	1:B:443:PRO:HD3	1.85	0.41
1:B:378:ASP:O	1:B:379:ASN:HB2	2.19	0.41
1:A:251:ASP:HA	1:A:252:PRO:HD3	1.74	0.41
1:A:310:ALA:O	2:A:893:HOH:O	2.22	0.41
1:A:374:THR:HG23	1:A:381:THR:HG22	2.02	0.41
1:A:74:LEU:O	1:A:78:GLN:HG3	2.21	0.41
1:A:144:LYS:NZ	2:A:661:HOH:O	2.53	0.41
1:A:497:THR:HG23	1:B:156:GLN:HE21	1.86	0.41
1:A:71:THR:HB	2:A:809:HOH:O	2.21	0.41
1:B:363:LYS:HE2	1:B:365:VAL:CG2	2.51	0.41
1:B:363:LYS:HE2	1:B:365:VAL:HG21	2.02	0.41
1:A:71:THR:CB	2:A:809:HOH:O	2.69	0.41
1:A:286:ARG:HD3	2:A:907:HOH:O	2.21	0.40
1:A:173:LYS:NZ	2:A:606:HOH:O	2.35	0.40
1:B:111:SER:HB3	1:B:135:LYS:HD2	2.03	0.40
1:B:208:LEU:HD12	1:B:208:LEU:C	2.46	0.40
1:B:491:LEU:HA	1:B:491:LEU:HD23	1.86	0.40
1:B:184:ARG:CD	2:B:904:HOH:O	2.69	0.40
1:B:204:LEU:HD12	1:B:204:LEU:HA	1.79	0.40
1:A:437:SER:HG	1:A:453:ARG:HB2	1.86	0.40
1:B:73:GLN:HG2	1:B:505:LEU:CD1	2.51	0.40
1:B:351:VAL:HG22	1:B:397:LEU:HD23	2.03	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:834:HOH:O	2:B:756:HOH:O[3_545]	1.79	0.41
2:A:712:HOH:O	2:B:788:HOH:O[4_555]	1.84	0.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:801:HOH:O	2:B:887:HOH:O[3_555]	1.90	0.30
2:A:682:HOH:O	2:A:725:HOH:O[2_555]	2.15	0.05

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	423/463 (91%)	409 (97%)	14 (3%)	0	100	100
1	B	419/463 (90%)	407 (97%)	11 (3%)	1 (0%)	43	44
All	All	842/926 (91%)	816 (97%)	25 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	317	ASP

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	359/385 (93%)	337 (94%)	22 (6%)	17	15
1	B	356/385 (92%)	338 (95%)	18 (5%)	21	21
All	All	715/770 (93%)	675 (94%)	40 (6%)	19	18

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	98	LEU
1	A	103	SER
1	A	105	LEU
1	A	106	SER
1	A	110	GLN
1	A	111	SER
1	A	117	GLN
1	A	132	LEU
1	A	170	ASN
1	A	198	LEU
1	A	218	VAL
1	A	220	ASP
1	A	223	THR
1	A	262	GLU
1	A	331	SER
1	A	406	GLN
1	A	437	SER
1	A	440	LYS
1	A	441	LEU
1	A	462	GLN
1	A	470	ASN
1	B	79	ASN
1	B	92	SER
1	B	102	SER
1	B	170	ASN
1	B	184	ARG
1	B	203	GLN
1	B	204	LEU
1	B	208	LEU
1	B	217	SER
1	B	262	GLU
1	B	275	ASN
1	B	290	LEU
1	B	302	LEU
1	B	397	LEU
1	B	401	VAL
1	B	441	LEU
1	B	504	GLN
1	B	509	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	73	GLN
1	A	78	GLN
1	A	117	GLN
1	A	141	ASN
1	A	142	GLN
1	A	148	GLN
1	A	167	GLN
1	A	219	GLN
1	A	225	ASN
1	A	242	GLN
1	A	408	ASN
1	A	424	ASN
1	A	462	GLN
1	A	465	ASN
1	A	470	ASN
1	B	90	GLN
1	B	96	ASN
1	B	110	GLN
1	B	142	GLN
1	B	153	GLN
1	B	170	ASN
1	B	174	GLN
1	B	219	GLN
1	B	225	ASN
1	B	266	ASN
1	B	275	ASN
1	B	339	ASN
1	B	358	GLN
1	B	465	ASN
1	B	486	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 [i](#)

There are no oligosaccharides 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

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	429/463 (92%)	0.39	24 (5%) 30 32	23, 36, 62, 81	0
1	B	425/463 (91%)	0.60	38 (8%) 15 16	26, 39, 69, 100	0
All	All	854/926 (92%)	0.49	62 (7%) 21 22	23, 37, 66, 100	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	ASP	4.9
1	B	103	SER	4.9
1	B	509	GLN	4.6
1	B	506	TYR	4.5
1	B	70	ILE	4.2
1	A	441	LEU	4.2
1	A	70	ILE	4.1
1	B	72	ASN	4.0
1	B	502	VAL	4.0
1	B	441	LEU	3.9
1	B	505	LEU	3.7
1	B	443	PRO	3.5
1	A	69	PHE	3.4
1	B	197	LEU	3.4
1	B	102	SER	3.3
1	A	221	GLY	3.2
1	A	507	LYS	3.2
1	B	203	GLN	3.1
1	B	436	ALA	3.1
1	B	439	SER	3.1
1	A	68	ALA	3.1
1	B	74	LEU	3.0
1	B	384	ALA	3.0
1	A	98	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	197	LEU	2.9
1	B	222	GLY	2.9
1	B	170	ASN	2.9
1	A	511	SER	2.8
1	B	451	ASP	2.8
1	A	438	GLU	2.7
1	A	196	ASP	2.7
1	B	199	ASP	2.7
1	B	184	ARG	2.6
1	B	185	MET	2.6
1	A	67	ASP	2.6
1	B	196	ASP	2.6
1	A	368	GLY	2.6
1	B	508	GLN	2.5
1	A	185	MET	2.5
1	B	453	ARG	2.5
1	B	124	GLU	2.5
1	A	344	THR	2.5
1	B	183	SER	2.5
1	B	71	THR	2.4
1	B	437	SER	2.4
1	B	450	SER	2.3
1	A	388	ALA	2.3
1	B	275	ASN	2.3
1	B	75	ARG	2.3
1	A	505	LEU	2.3
1	A	102	SER	2.2
1	B	198	LEU	2.2
1	B	104	SER	2.2
1	A	186	THR	2.2
1	B	122	ASN	2.2
1	B	167	GLN	2.1
1	B	499	ALA	2.1
1	A	198	LEU	2.1
1	A	105	LEU	2.1
1	A	203	GLN	2.0
1	A	402	GLY	2.0
1	B	200	GLN	2.0

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

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.