



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:16 AM GMT

PDB ID : 3A5I
Title : Structure of the cytoplasmic domain of FlhA
Authors : Imada, K.; Saijo-Hamano, Y.; Shimada, M.; Namba, K.
Deposited on : 2009-08-07
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

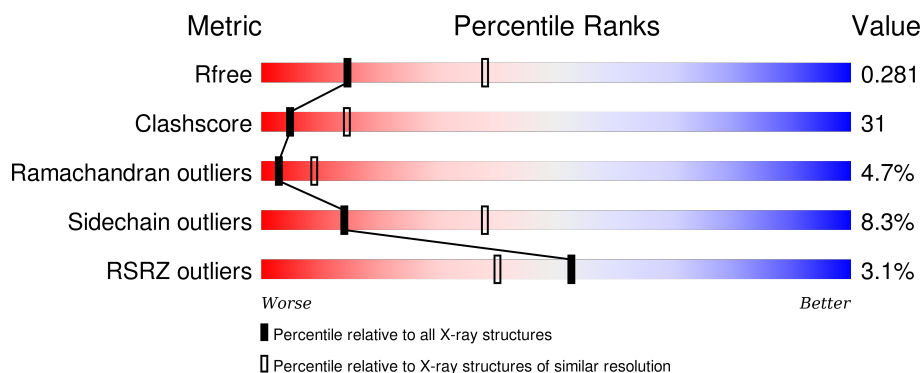
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	389	
1	B	389	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5336 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 biosynthesis protein flhA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2681	1695	478	499	9			
1	B	342	Total	C	N	O	S	0	0	0
			2655	1681	472	493	9			

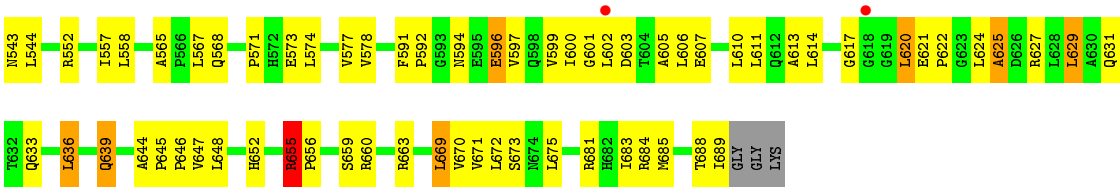
There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	304	MET	-	EXPRESSION TAG	UNP P40729
A	305	GLY	-	EXPRESSION TAG	UNP P40729
A	306	HIS	-	EXPRESSION TAG	UNP P40729
A	307	HIS	-	EXPRESSION TAG	UNP P40729
A	308	HIS	-	EXPRESSION TAG	UNP P40729
A	309	HIS	-	EXPRESSION TAG	UNP P40729
A	310	HIS	-	EXPRESSION TAG	UNP P40729
A	311	HIS	-	EXPRESSION TAG	UNP P40729
A	312	HIS	-	EXPRESSION TAG	UNP P40729
A	313	HIS	-	EXPRESSION TAG	UNP P40729
A	314	HIS	-	EXPRESSION TAG	UNP P40729
A	315	HIS	-	EXPRESSION TAG	UNP P40729
A	316	SER	-	EXPRESSION TAG	UNP P40729
A	317	SER	-	EXPRESSION TAG	UNP P40729
A	318	GLY	-	EXPRESSION TAG	UNP P40729
A	319	HIS	-	EXPRESSION TAG	UNP P40729
A	320	ILE	-	EXPRESSION TAG	UNP P40729
A	321	ASP	-	EXPRESSION TAG	UNP P40729
A	322	ASP	-	EXPRESSION TAG	UNP P40729
A	323	ASP	-	EXPRESSION TAG	UNP P40729
A	324	ASP	-	EXPRESSION TAG	UNP P40729
A	325	LYS	-	EXPRESSION TAG	UNP P40729
A	326	HIS	-	EXPRESSION TAG	UNP P40729
A	327	MET	-	EXPRESSION TAG	UNP P40729
B	304	MET	-	EXPRESSION TAG	UNP P40729

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Chain	Residue	Modelled	Actual	Comment	Reference
B	305	GLY	-	EXPRESSION TAG	UNP P40729
B	306	HIS	-	EXPRESSION TAG	UNP P40729
B	307	HIS	-	EXPRESSION TAG	UNP P40729
B	308	HIS	-	EXPRESSION TAG	UNP P40729
B	309	HIS	-	EXPRESSION TAG	UNP P40729
B	310	HIS	-	EXPRESSION TAG	UNP P40729
B	311	HIS	-	EXPRESSION TAG	UNP P40729
B	312	HIS	-	EXPRESSION TAG	UNP P40729
B	313	HIS	-	EXPRESSION TAG	UNP P40729
B	314	HIS	-	EXPRESSION TAG	UNP P40729
B	315	HIS	-	EXPRESSION TAG	UNP P40729
B	316	SER	-	EXPRESSION TAG	UNP P40729
B	317	SER	-	EXPRESSION TAG	UNP P40729
B	318	GLY	-	EXPRESSION TAG	UNP P40729
B	319	HIS	-	EXPRESSION TAG	UNP P40729
B	320	ILE	-	EXPRESSION TAG	UNP P40729
B	321	ASP	-	EXPRESSION TAG	UNP P40729
B	322	ASP	-	EXPRESSION TAG	UNP P40729
B	323	ASP	-	EXPRESSION TAG	UNP P40729
B	324	ASP	-	EXPRESSION TAG	UNP P40729
B	325	LYS	-	EXPRESSION TAG	UNP P40729
B	326	HIS	-	EXPRESSION TAG	UNP P40729
B	327	MET	-	EXPRESSION TAG	UNP P40729



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	216.32Å 216.32Å 65.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.80 – 2.80 40.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.80-2.80) 99.6 (40.84-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.257 , 0.290 0.251 , 0.281	Depositor DCC
R_{free} test set	1862 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	73.5	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.3	EDS
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 37317 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5336	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.40	0/2727	0.65	0/3703
1	B	0.43	0/2701	0.67	1/3671 (0.0%)
All	All	0.42	0/5428	0.66	1/7374 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	451	GLY	N-CA-C	5.07	125.77	113.10

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	2681	0	2740	211	0
1	B	2655	0	2715	139	0
All	All	5336	0	5455	339	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 31.

All (339) 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:376:ASP:CB	1:A:379:GLN:HE21	1.36	1.37
1:A:373:PRO:HA	1:A:379:GLN:HE22	1.08	1.10
1:A:376:ASP:HB2	1:A:379:GLN:HE21	0.96	1.09
1:A:511:GLN:NE2	1:B:354:TRP:HE1	1.49	1.09
1:A:376:ASP:CB	1:A:379:GLN:NE2	2.19	1.03
1:A:688:THR:HG22	1:A:689:ILE:H	1.21	1.02
1:B:450:PRO:HD2	1:B:470:LEU:HD21	1.37	1.02
1:A:376:ASP:HB2	1:A:379:GLN:NE2	1.76	0.99
1:B:466:ILE:HG22	1:B:467:GLU:H	1.30	0.95
1:B:473:GLN:HE21	1:B:477:GLN:HE21	1.10	0.95
1:A:600:ILE:HG13	1:A:639:GLN:HE21	1.32	0.95
1:A:376:ASP:HB3	1:A:379:GLN:HG3	1.50	0.94
1:B:440:ILE:HD11	1:B:461:LEU:HB2	1.45	0.94
1:A:376:ASP:HB3	1:A:379:GLN:HE21	1.32	0.92
1:A:568:GLN:NE2	1:A:573:GLU:HG2	1.86	0.91
1:A:373:PRO:HA	1:A:379:GLN:NE2	1.90	0.86
1:B:603:ASP:HB3	1:B:606:LEU:HD23	1.58	0.86
1:A:579:ARG:HH21	1:A:655:ARG:CZ	1.89	0.86
1:B:450:PRO:HD2	1:B:470:LEU:CD2	2.08	0.84
1:A:674:ASN:ND2	1:A:675:LEU:HD12	1.92	0.84
1:A:511:GLN:NE2	1:B:354:TRP:NE1	2.23	0.82
1:B:629:LEU:O	1:B:633:GLN:HG3	1.80	0.82
1:B:473:GLN:HE21	1:B:477:GLN:NE2	1.78	0.81
1:B:601:GLY:HA3	1:B:685:MET:SD	2.22	0.79
1:B:627:ARG:HH11	1:B:627:ARG:HG2	1.48	0.79
1:A:376:ASP:HB3	1:A:379:GLN:CG	2.13	0.78
1:B:688:THR:HG22	1:B:689:ILE:H	1.48	0.78
1:A:390:ILE:HD13	1:A:493:ASN:HB2	1.66	0.78
1:A:376:ASP:HB3	1:A:379:GLN:NE2	1.93	0.78
1:A:380:ASP:C	1:A:380:ASP:OD1	2.22	0.78
1:A:606:LEU:HA	1:A:609:LEU:HD12	1.67	0.77
1:B:621:GLU:HG3	1:B:622:PRO:HD2	1.64	0.77
1:A:539:LYS:HE3	1:A:543:ASN:HD21	1.49	0.77
1:B:461:LEU:H	1:B:461:LEU:HD22	1.50	0.76
1:B:596:GLU:HG3	1:B:684:ARG:HH11	1.51	0.75
1:B:472:GLU:HA	1:B:475:GLN:HE21	1.51	0.75
1:B:536:THR:HG22	1:B:571:PRO:HG3	1.69	0.74
1:A:688:THR:HG22	1:A:689:ILE:N	1.99	0.74
1:B:440:ILE:HG23	1:B:480:THR:OG1	1.87	0.74
1:A:453:LYS:H	1:A:453:LYS:HD2	1.51	0.74
1:A:637:SER:HA	1:A:640:GLU:HB2	1.70	0.73
1:A:451:GLY:HA3	1:A:465:TRP:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:LEU:H	1:A:470:LEU:HD12	1.51	0.73
1:A:507:GLN:O	1:A:511:GLN:HG3	1.88	0.72
1:B:419:ARG:HD2	1:B:426:GLU:OE1	1.90	0.72
1:A:531:VAL:HG12	1:A:565:ALA:HB3	1.72	0.71
1:A:655:ARG:HG2	1:A:671:VAL:HG12	1.72	0.70
1:A:688:THR:CG2	1:A:689:ILE:H	2.01	0.70
1:A:607:GLU:O	1:A:611:LEU:HB2	1.91	0.70
1:A:601:GLY:O	1:A:688:THR:HA	1.91	0.70
1:B:594:ASN:HA	1:B:681:ARG:NH1	2.07	0.70
1:A:510:GLN:HG2	1:A:534:LEU:HD11	1.72	0.70
1:A:473:GLN:O	1:A:476:ILE:HG12	1.91	0.70
1:A:419:ARG:HD2	1:A:426:GLU:OE1	1.92	0.70
1:A:375:VAL:CG2	1:A:407:ILE:HD13	2.22	0.70
1:B:688:THR:HG22	1:B:689:ILE:N	2.07	0.69
1:A:657:LEU:H	1:A:657:LEU:HD23	1.57	0.69
1:B:594:ASN:HA	1:B:681:ARG:HH12	1.56	0.69
1:B:621:GLU:CG	1:B:622:PRO:HD2	2.23	0.68
1:A:367:VAL:HG22	1:A:371:LEU:HB2	1.75	0.68
1:A:522:LYS:HB2	1:B:507:GLN:OE1	1.93	0.67
1:B:627:ARG:O	1:B:631:GLN:HG3	1.95	0.67
1:A:654:LEU:HD13	1:A:658:LEU:HD11	1.76	0.67
1:A:663:ARG:C	1:A:665:SER:H	1.97	0.67
1:A:420:ILE:HD13	1:A:492:LEU:HD23	1.76	0.66
1:B:670:VAL:HG12	1:B:672:LEU:HD13	1.78	0.66
1:A:379:GLN:O	1:A:380:ASP:C	2.34	0.65
1:B:528:VAL:HG12	1:B:532:VAL:O	1.97	0.65
1:B:596:GLU:HG3	1:B:684:ARG:NH1	2.11	0.65
1:A:623:GLY:O	1:A:627:ARG:HG2	1.97	0.64
1:A:373:PRO:CA	1:A:379:GLN:HE22	1.99	0.64
1:A:527:LEU:HD12	1:A:531:VAL:HB	1.78	0.64
1:A:659:SER:O	1:A:663:ARG:HG3	1.98	0.64
1:B:466:ILE:HG22	1:B:467:GLU:N	2.09	0.63
1:B:445:ALA:CB	1:B:478:GLY:HA3	2.28	0.63
1:A:603:ASP:HB3	1:A:606:LEU:CB	2.27	0.63
1:A:600:ILE:HD11	1:A:639:GLN:HG3	1.79	0.63
1:A:463:ALA:C	1:A:464:ILE:HD12	2.19	0.63
1:B:601:GLY:O	1:B:688:THR:HA	1.98	0.63
1:A:470:LEU:CD1	1:A:470:LEU:H	2.13	0.62
1:B:659:SER:O	1:B:663:ARG:HG3	2.00	0.62
1:B:388:ARG:HH11	1:B:388:ARG:HG2	1.63	0.62
1:A:401:LEU:HD11	1:B:352:ALA:HB1	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ASN:HB2	1:A:479:PHE:HE2	1.63	0.62
1:B:472:GLU:O	1:B:476:ILE:HG12	1.98	0.61
1:A:646:PRO:O	1:A:669:LEU:HD12	2.00	0.61
1:A:391:ARG:NH1	1:A:402:PRO:O	2.33	0.61
1:A:579:ARG:HH21	1:A:655:ARG:NE	1.98	0.61
1:B:507:GLN:O	1:B:511:GLN:HG3	1.99	0.61
1:A:373:PRO:O	1:A:379:GLN:NE2	2.34	0.60
1:A:674:ASN:HD22	1:A:675:LEU:HD12	1.66	0.60
1:A:627:ARG:HH11	1:A:627:ARG:HG3	1.66	0.60
1:A:445:ALA:HB2	1:A:478:GLY:HA3	1.83	0.60
1:B:647:VAL:HG11	1:B:672:LEU:HD22	1.82	0.60
1:B:445:ALA:HB3	1:B:478:GLY:O	2.00	0.60
1:B:620:LEU:N	1:B:620:LEU:HD12	2.15	0.60
1:B:393:LYS:HE2	1:B:397:ASP:OD2	2.01	0.60
1:A:654:LEU:HB3	1:A:658:LEU:CD1	2.32	0.60
1:A:390:ILE:HG23	1:A:493:ASN:HD22	1.67	0.60
1:A:603:ASP:HB3	1:A:606:LEU:HB3	1.82	0.60
1:A:473:GLN:HA	1:A:476:ILE:HG12	1.83	0.60
1:A:445:ALA:CB	1:A:478:GLY:HA3	2.32	0.60
1:B:466:ILE:CG2	1:B:470:LEU:HB3	2.32	0.60
1:A:645:PRO:HB2	1:A:647:VAL:HG23	1.84	0.60
1:A:375:VAL:HG13	1:A:375:VAL:O	2.01	0.59
1:A:655:ARG:HB3	1:A:656:PRO:HD3	1.83	0.59
1:A:674:ASN:HD21	1:A:675:LEU:HD12	1.67	0.59
1:A:453:LYS:N	1:A:453:LYS:HD2	2.15	0.59
1:A:441:ASN:ND2	1:A:443:GLY:H	2.00	0.59
1:A:513:LEU:HD23	1:A:537:LEU:CD2	2.32	0.59
1:B:377:PHE:HD1	1:B:378:GLN:HG3	1.67	0.58
1:B:394:PHE:CD2	1:B:402:PRO:HG3	2.37	0.58
1:B:639:GLN:HE21	1:B:639:GLN:HA	1.67	0.58
1:A:374:MET:O	1:A:381:GLY:CA	2.52	0.58
1:A:520:MET:SD	1:A:523:LEU:HD12	2.43	0.58
1:A:511:GLN:HE22	1:B:354:TRP:HE1	1.47	0.57
1:B:391:ARG:NH1	1:B:402:PRO:O	2.37	0.57
1:B:533:THR:HG23	1:B:536:THR:H	1.70	0.57
1:A:470:LEU:N	1:A:470:LEU:HD12	2.18	0.57
1:B:602:LEU:HD23	1:B:602:LEU:H	1.70	0.57
1:B:350:VAL:HG22	1:B:351:GLU:N	2.20	0.56
1:A:367:VAL:HG22	1:A:371:LEU:CB	2.36	0.56
1:A:631:GLN:HG2	1:A:692:LYS:CE	2.34	0.56
1:A:536:THR:HG23	1:A:571:PRO:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:ARG:HA	1:B:538:HIS:CD2	2.41	0.56
1:A:350:VAL:HG22	1:A:351:GLU:N	2.20	0.55
1:B:461:LEU:N	1:B:461:LEU:HD22	2.19	0.55
1:B:639:GLN:NE2	1:B:644:ALA:HB3	2.21	0.55
1:B:611:LEU:O	1:B:614:LEU:HB2	2.06	0.55
1:B:482:VAL:HG23	1:B:487:VAL:HG12	1.89	0.55
1:A:565:ALA:HB3	1:A:566:PRO:HD3	1.89	0.55
1:A:502:GLU:N	1:A:502:GLU:OE2	2.34	0.54
1:A:417:ARG:HG3	1:A:418:TYR:N	2.21	0.54
1:A:440:ILE:HG23	1:A:480:THR:HB	1.88	0.54
1:A:440:ILE:HD12	1:A:456:ASP:HB2	1.89	0.54
1:A:597:VAL:HB	1:A:683:ILE:HD13	1.89	0.54
1:A:568:GLN:HE21	1:A:573:GLU:HG2	1.65	0.54
1:A:674:ASN:ND2	1:A:675:LEU:CD1	2.69	0.54
1:A:376:ASP:CB	1:A:379:GLN:HG3	2.31	0.54
1:A:383:LEU:HD11	1:A:488:VAL:HG11	1.89	0.54
1:B:521:PRO:O	1:B:525:GLU:HG3	2.08	0.54
1:A:370:ARG:HG2	1:A:370:ARG:HH11	1.73	0.53
1:B:470:LEU:HD12	1:B:473:GLN:HB3	1.89	0.53
1:B:683:ILE:HD12	1:B:683:ILE:N	2.23	0.53
1:B:390:ILE:HD12	1:B:493:ASN:HB2	1.90	0.53
1:A:674:ASN:HD21	1:A:675:LEU:CD1	2.22	0.53
1:A:376:ASP:CB	1:A:379:GLN:CG	2.84	0.53
1:A:375:VAL:HG21	1:A:407:ILE:HG21	1.90	0.53
1:A:602:LEU:H	1:A:602:LEU:HD23	1.72	0.53
1:B:531:VAL:HG12	1:B:565:ALA:HB3	1.91	0.53
1:B:466:ILE:HG23	1:B:470:LEU:HD23	1.90	0.53
1:A:370:ARG:HB2	1:A:415:PRO:O	2.08	0.53
1:B:636:LEU:O	1:B:636:LEU:HD13	2.08	0.53
1:A:518:GLN:O	1:A:518:GLN:HG3	2.08	0.53
1:A:380:ASP:OD1	1:A:380:ASP:O	2.27	0.53
1:B:472:GLU:HA	1:B:475:GLN:NE2	2.21	0.53
1:A:533:THR:CG2	1:A:536:THR:H	2.22	0.52
1:B:655:ARG:HG2	1:B:671:VAL:HG12	1.91	0.52
1:A:620:LEU:N	1:A:620:LEU:HD23	2.24	0.52
1:A:651:ASN:HA	1:A:674:ASN:OD1	2.10	0.52
1:B:627:ARG:HH11	1:B:627:ARG:CG	2.19	0.52
1:A:392:LYS:HZ2	1:B:348:SER:HB3	1.74	0.52
1:A:600:ILE:HG12	1:A:687:ALA:HB3	1.92	0.52
1:A:579:ARG:HE	1:A:655:ARG:NH1	2.07	0.52
1:B:688:THR:CG2	1:B:689:ILE:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:ILE:HG13	1:B:639:GLN:OE1	2.09	0.52
1:B:534:LEU:O	1:B:534:LEU:HD22	2.10	0.52
1:A:432:ALA:O	1:A:434:PRO:HD3	2.10	0.51
1:A:372:ILE:N	1:A:373:PRO:CD	2.74	0.51
1:A:602:LEU:H	1:A:602:LEU:CD2	2.24	0.51
1:A:689:ILE:O	1:A:689:ILE:HG22	2.10	0.51
1:A:441:ASN:HB2	1:A:479:PHE:CE2	2.45	0.51
1:A:442:PRO:HA	1:A:461:LEU:HD23	1.91	0.51
1:A:600:ILE:HG13	1:A:639:GLN:NE2	2.15	0.51
1:A:390:ILE:CD1	1:A:493:ASN:HB2	2.40	0.51
1:A:392:LYS:NZ	1:B:348:SER:HB3	2.26	0.51
1:A:531:VAL:HG12	1:A:565:ALA:CB	2.41	0.50
1:A:474:ALA:O	1:A:479:PHE:HB2	2.11	0.50
1:B:438:LEU:HD13	1:B:465:TRP:CE2	2.47	0.50
1:A:376:ASP:HB3	1:A:379:GLN:CD	2.32	0.50
1:B:440:ILE:HD12	1:B:463:ALA:HB2	1.92	0.50
1:A:603:ASP:HB3	1:A:606:LEU:HB2	1.93	0.50
1:B:655:ARG:HB3	1:B:656:PRO:HD3	1.94	0.50
1:A:684:ARG:O	1:A:686:THR:HG23	2.12	0.50
1:A:392:LYS:HG3	1:B:352:ALA:HB2	1.93	0.50
1:B:600:ILE:HD11	1:B:639:GLN:HG3	1.93	0.50
1:A:638:ARG:O	1:A:642:LEU:HG	2.11	0.50
1:B:627:ARG:NH1	1:B:627:ARG:HG2	2.23	0.50
1:A:444:THR:OG1	1:A:445:ALA:N	2.42	0.50
1:B:482:VAL:CG2	1:B:487:VAL:HG12	2.42	0.50
1:B:445:ALA:HB1	1:B:478:GLY:HA3	1.93	0.50
1:A:471:LYS:HG2	1:A:475:GLN:NE2	2.27	0.50
1:B:574:LEU:O	1:B:578:VAL:HG23	2.12	0.50
1:A:375:VAL:HG21	1:A:407:ILE:HD13	1.92	0.49
1:A:591:PHE:N	1:A:592:PRO:HD3	2.25	0.49
1:B:440:ILE:HD13	1:B:456:ASP:HB2	1.94	0.49
1:A:649:LEU:HD23	1:A:677:LEU:HD23	1.94	0.49
1:A:684:ARG:HD2	1:A:686:THR:HG22	1.94	0.49
1:A:684:ARG:O	1:A:686:THR:N	2.42	0.49
1:A:453:LYS:H	1:A:453:LYS:CD	2.21	0.49
1:A:600:ILE:HG22	1:A:648:LEU:HD13	1.95	0.49
1:A:450:PRO:HG2	1:A:470:LEU:HD21	1.94	0.49
1:A:600:ILE:CD1	1:A:639:GLN:HG3	2.44	0.48
1:A:663:ARG:C	1:A:665:SER:N	2.66	0.48
1:B:574:LEU:O	1:B:577:VAL:HG22	2.13	0.48
1:B:466:ILE:HG22	1:B:470:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:ARG:HD2	1:A:686:THR:CG2	2.44	0.48
1:A:376:ASP:OD1	1:A:379:GLN:HG2	2.13	0.48
1:A:438:LEU:HD13	1:A:465:TRP:CE2	2.49	0.48
1:A:375:VAL:HG22	1:A:407:ILE:HD13	1.96	0.48
1:B:591:PHE:N	1:B:592:PRO:HD3	2.28	0.48
1:A:524:THR:OG1	1:A:525:GLU:N	2.46	0.48
1:A:652:HIS:HB2	1:A:675:LEU:HD13	1.96	0.48
1:A:622:PRO:O	1:A:624:LEU:N	2.47	0.48
1:A:524:THR:O	1:A:527:LEU:N	2.44	0.47
1:A:631:GLN:HG2	1:A:692:LYS:NZ	2.29	0.47
1:A:538:HIS:CE1	1:A:542:GLN:NE2	2.81	0.47
1:B:440:ILE:HG22	1:B:480:THR:O	2.14	0.47
1:A:450:PRO:O	1:A:451:GLY:O	2.32	0.47
1:A:473:GLN:HA	1:A:476:ILE:CD1	2.44	0.47
1:B:645:PRO:C	1:B:647:VAL:H	2.17	0.47
1:A:469:ALA:O	1:A:471:LYS:N	2.48	0.47
1:B:539:LYS:O	1:B:543:ASN:ND2	2.45	0.47
1:B:507:GLN:HA	1:B:507:GLN:NE2	2.29	0.47
1:A:370:ARG:NH2	1:A:434:PRO:HD2	2.29	0.47
1:B:474:ALA:O	1:B:479:PHE:HB2	2.15	0.47
1:B:461:LEU:H	1:B:461:LEU:CD2	2.23	0.47
1:A:591:PHE:CE2	1:A:597:VAL:HG13	2.50	0.47
1:B:417:ARG:HH21	1:B:431:ASP:CG	2.18	0.47
1:B:652:HIS:HA	1:B:673:SER:HB2	1.97	0.47
1:B:379:GLN:NE2	1:B:381:GLY:H	2.13	0.47
1:B:607:GLU:O	1:B:611:LEU:HG	2.15	0.47
1:B:596:GLU:CG	1:B:684:ARG:HD3	2.45	0.46
1:A:388:ARG:HG2	1:B:351:GLU:OE2	2.15	0.46
1:B:390:ILE:HG23	1:B:493:ASN:OD1	2.15	0.46
1:B:597:VAL:HG12	1:B:599:VAL:HG13	1.97	0.46
1:A:445:ALA:HB2	1:A:478:GLY:CA	2.46	0.46
1:B:365:MET:HA	1:B:419:ARG:O	2.15	0.46
1:A:513:LEU:HD23	1:A:537:LEU:HD21	1.97	0.46
1:A:645:PRO:HA	1:A:646:PRO:HD3	1.73	0.46
1:B:568:GLN:NE2	1:B:573:GLU:HG3	2.31	0.46
1:B:410:ASN:HD21	1:B:412:ASP:HB2	1.79	0.46
1:B:463:ALA:C	1:B:464:ILE:HG13	2.35	0.46
1:B:396:GLN:O	1:B:552:ARG:HD2	2.16	0.46
1:B:652:HIS:CG	1:B:675:LEU:HD12	2.50	0.46
1:B:439:ALA:HB2	1:B:466:ILE:CG1	2.46	0.46
1:A:576:ALA:O	1:A:579:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:PHE:CE1	1:B:645:PRO:HG2	2.50	0.45
1:A:445:ALA:HB2	1:A:478:GLY:C	2.36	0.45
1:A:637:SER:O	1:A:641:MET:HG3	2.17	0.45
1:A:528:VAL:HG23	1:A:529:PRO:HA	1.98	0.45
1:B:444:THR:OG1	1:B:445:ALA:N	2.50	0.45
1:A:600:ILE:CG1	1:A:639:GLN:HG3	2.47	0.45
1:A:654:LEU:O	1:A:657:LEU:HD23	2.16	0.45
1:A:624:LEU:O	1:A:627:ARG:HB2	2.16	0.45
1:A:533:THR:HG23	1:A:536:THR:H	1.82	0.45
1:A:605:ALA:O	1:A:609:LEU:HG	2.17	0.45
1:B:421:LEU:HB3	1:B:426:GLU:HA	1.98	0.45
1:B:639:GLN:HE21	1:B:639:GLN:CA	2.27	0.45
1:A:668:GLN:HG2	1:A:668:GLN:O	2.17	0.44
1:A:654:LEU:HB3	1:A:658:LEU:HD12	1.99	0.44
1:A:400:PHE:HA	1:B:354:TRP:CZ3	2.52	0.44
1:A:515:ARG:O	1:A:518:GLN:HG2	2.17	0.44
1:A:377:PHE:HD1	1:A:378:GLN:H	1.65	0.44
1:B:536:THR:O	1:B:540:VAL:HG23	2.18	0.44
1:A:369:TYR:HA	1:A:372:ILE:HG13	1.99	0.44
1:A:367:VAL:CG2	1:A:371:LEU:HB3	2.47	0.44
1:A:469:ALA:C	1:A:471:LYS:H	2.21	0.44
1:A:418:TYR:CE2	1:A:488:VAL:HG22	2.53	0.44
1:A:394:PHE:HZ	1:A:497:GLY:HA2	1.82	0.44
1:B:363:LEU:HD23	1:B:405:VAL:HG22	1.99	0.43
1:A:376:ASP:CG	1:A:379:GLN:CG	2.86	0.43
1:A:417:ARG:HG3	1:A:418:TYR:H	1.82	0.43
1:B:441:ASN:ND2	1:B:445:ALA:O	2.37	0.43
1:B:557:ILE:HG23	1:B:578:VAL:HG11	1.99	0.43
1:A:649:LEU:HD13	1:A:650:VAL:N	2.33	0.43
1:B:596:GLU:HB2	1:B:684:ARG:HD3	2.00	0.43
1:A:388:ARG:HD2	1:B:350:VAL:O	2.19	0.43
1:A:367:VAL:CG2	1:A:371:LEU:CB	2.97	0.43
1:B:645:PRO:HA	1:B:646:PRO:HD3	1.76	0.43
1:B:459:PHE:HB2	1:B:461:LEU:CD2	2.49	0.43
1:B:656:PRO:O	1:B:660:ARG:HG3	2.19	0.43
1:A:456:ASP:HA	1:A:457:PRO:HD3	1.88	0.43
1:B:573:GLU:OE2	1:B:573:GLU:HA	2.19	0.43
1:B:610:LEU:O	1:B:613:ALA:HB3	2.19	0.43
1:A:521:PRO:O	1:A:525:GLU:HG2	2.19	0.42
1:A:371:LEU:HD13	1:A:416:ALA:HA	2.00	0.42
1:B:646:PRO:O	1:B:669:LEU:HD23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:LEU:HG	1:B:567:LEU:O	2.19	0.42
1:A:450:PRO:HD2	1:A:470:LEU:HD23	2.01	0.42
1:A:597:VAL:HG12	1:A:599:VAL:HG13	2.01	0.42
1:B:603:ASP:OD2	1:B:605:ALA:HB3	2.19	0.42
1:A:525:GLU:OE1	1:A:525:GLU:HA	2.18	0.42
1:A:574:LEU:O	1:A:578:VAL:HG23	2.19	0.42
1:A:593:GLY:O	1:A:681:ARG:NH1	2.44	0.42
1:A:473:GLN:CA	1:A:476:ILE:HG12	2.49	0.42
1:B:350:VAL:HG22	1:B:351:GLU:H	1.85	0.42
1:B:577:VAL:HG23	1:B:578:VAL:N	2.35	0.42
1:B:502:GLU:OE1	1:B:502:GLU:N	2.44	0.42
1:A:547:GLU:O	1:A:548:LYS:HB2	2.17	0.42
1:A:513:LEU:O	1:A:513:LEU:HD13	2.19	0.42
1:A:631:GLN:O	1:A:634:GLU:HB3	2.19	0.42
1:B:527:LEU:HD23	1:B:558:LEU:HD22	2.01	0.42
1:B:620:LEU:H	1:B:620:LEU:HD12	1.82	0.42
1:B:624:LEU:O	1:B:625:ALA:C	2.58	0.42
1:B:361:ASP:O	1:B:423:LYS:HA	2.19	0.42
1:B:372:ILE:N	1:B:373:PRO:CD	2.83	0.42
1:A:674:ASN:HD22	1:A:675:LEU:N	2.18	0.41
1:A:473:GLN:HA	1:A:476:ILE:CG1	2.48	0.41
1:A:539:LYS:HE3	1:A:543:ASN:ND2	2.27	0.41
1:A:614:LEU:O	1:A:614:LEU:HD23	2.19	0.41
1:A:471:LYS:HG3	1:A:481:VAL:HG11	2.02	0.41
1:B:377:PHE:HD1	1:B:378:GLN:H	1.62	0.41
1:B:366:GLU:HA	1:B:408:ARG:O	2.21	0.41
1:A:380:ASP:CG	1:A:380:ASP:O	2.59	0.41
1:A:441:ASN:HA	1:A:442:PRO:HD3	1.94	0.41
1:B:536:THR:HG22	1:B:571:PRO:CG	2.47	0.41
1:A:353:THR:O	1:A:356:ASP:HB2	2.21	0.41
1:A:454:THR:OG1	1:A:455:VAL:N	2.52	0.41
1:A:577:VAL:O	1:A:580:VAL:HG13	2.20	0.41
1:A:399:GLY:O	1:A:400:PHE:HB3	2.21	0.41
1:A:401:LEU:HA	1:A:402:PRO:HD3	1.96	0.41
1:A:645:PRO:C	1:A:647:VAL:H	2.24	0.41
1:B:600:ILE:HG22	1:B:648:LEU:HD13	2.02	0.41
1:A:374:MET:O	1:A:381:GLY:HA2	2.21	0.41
1:A:631:GLN:NE2	1:A:692:LYS:HE3	2.36	0.41
1:A:351:GLU:HG3	1:A:352:ALA:N	2.36	0.41
1:B:596:GLU:H	1:B:596:GLU:CD	2.24	0.41
1:A:464:ILE:N	1:A:464:ILE:HD12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:LYS:O	1:A:396:GLN:HG2	2.21	0.41
1:B:531:VAL:HG12	1:B:565:ALA:CB	2.51	0.41
1:B:379:GLN:HE21	1:B:379:GLN:HB3	1.62	0.41
1:B:459:PHE:CD1	1:B:459:PHE:N	2.89	0.40
1:A:621:GLU:HA	1:A:622:PRO:HD3	1.93	0.40
1:A:668:GLN:HB3	1:A:668:GLN:HE21	1.58	0.40
1:A:631:GLN:O	1:A:634:GLU:N	2.52	0.40
1:A:370:ARG:HH21	1:A:434:PRO:HD2	1.86	0.40
1:A:359:LEU:CD1	1:A:359:LEU:N	2.85	0.40
1:A:617:GLY:C	1:A:619:GLY:H	2.25	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	344/389 (88%)	294 (86%)	29 (8%)	21 (6%)	2	5
1	B	340/389 (87%)	296 (87%)	33 (10%)	11 (3%)	5	17
All	All	684/778 (88%)	590 (86%)	62 (9%)	32 (5%)	3	9

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	445	ALA
1	A	450	PRO
1	A	451	GLY
1	A	470	LEU
1	A	525	GLU
1	A	622	PRO
1	B	450	PRO
1	B	451	GLY

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Mol	Chain	Res	Type
1	B	458	ALA
1	A	349	VAL
1	A	444	THR
1	A	524	THR
1	A	595	GLU
1	A	617	GLY
1	A	685	MET
1	B	522	LYS
1	B	530	GLY
1	A	378	GLN
1	A	458	ALA
1	A	655	ARG
1	A	686	THR
1	B	625	ALA
1	A	469	ALA
1	B	525	GLU
1	B	629	LEU
1	A	434	PRO
1	A	530	GLY
1	A	625	ALA
1	A	664	ARG
1	B	377	PHE
1	B	655	ARG
1	B	617	GLY

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	289/328 (88%)	260 (90%)	29 (10%)	9	27
1	B	287/328 (88%)	268 (93%)	19 (7%)	21	51
All	All	576/656 (88%)	528 (92%)	48 (8%)	14	38

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	VAL
1	A	375	VAL
1	A	377	PHE
1	A	380	ASP
1	A	383	LEU
1	A	394	PHE
1	A	400	PHE
1	A	409	ASP
1	A	413	LEU
1	A	436	ARG
1	A	440	ILE
1	A	441	ASN
1	A	500	SER
1	A	503	LEU
1	A	512	LEU
1	A	513	LEU
1	A	520	MET
1	A	525	GLU
1	A	534	LEU
1	A	544	LEU
1	A	573	GLU
1	A	580	VAL
1	A	582	LEU
1	A	649	LEU
1	A	655	ARG
1	A	674	ASN
1	A	677	LEU
1	A	679	ASP
1	A	680	ASN
1	B	379	GLN
1	B	383	LEU
1	B	388	ARG
1	B	397	ASP
1	B	400	PHE
1	B	456	ASP
1	B	461	LEU
1	B	487	VAL
1	B	495	LEU
1	B	498	GLN
1	B	512	LEU
1	B	534	LEU
1	B	544	LEU
1	B	596	GLU

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Mol	Chain	Res	Type
1	B	620	LEU
1	B	636	LEU
1	B	639	GLN
1	B	655	ARG
1	B	669	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	379	GLN
1	A	441	ASN
1	A	475	GLN
1	A	493	ASN
1	A	510	GLN
1	A	511	GLN
1	A	518	GLN
1	A	542	GLN
1	A	543	ASN
1	A	612	GLN
1	A	631	GLN
1	A	639	GLN
1	A	668	GLN
1	A	674	ASN
1	A	680	ASN
1	B	378	GLN
1	B	379	GLN
1	B	410	ASN
1	B	475	GLN
1	B	477	GLN
1	B	498	GLN
1	B	538	HIS
1	B	615	GLN
1	B	651	ASN

5.3.3 RNA ⓘ

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 carbohydrates 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	346/389 (88%)	0.19	15 (4%) 39 27	37, 74, 123, 137	0
1	B	342/389 (87%)	0.10	6 (1%) 71 61	33, 72, 114, 130	0
All	All	688/778 (88%)	0.14	21 (3%) 52 40	33, 73, 122, 137	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	692	LYS	5.6
1	B	479	PHE	3.4
1	A	347	ASN	3.4
1	A	658	LEU	3.3
1	A	642	LEU	3.2
1	A	690	GLY	3.1
1	A	615	GLN	2.9
1	B	451	GLY	2.9
1	B	449	LEU	2.8
1	B	602	LEU	2.6
1	A	691	GLY	2.5
1	A	379	GLN	2.3
1	B	618	GLY	2.3
1	A	689	ILE	2.2
1	B	464	ILE	2.2
1	A	618	GLY	2.2
1	A	594	ASN	2.2
1	A	641	MET	2.1
1	A	682	HIS	2.1
1	A	380	ASP	2.0
1	A	617	GLY	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 carbohydrates 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.