



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:16 AM UTC

PDB ID : 3A5I / pdb_00003a5i
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

<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

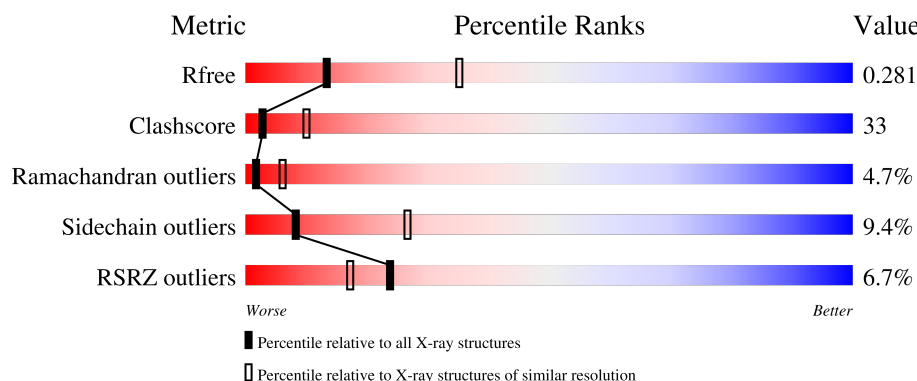
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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	389	7% 38% 41% 9% 11%
1	B	389	4% 45% 37% 6% 12%

2 Entry composition [i](#)

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			

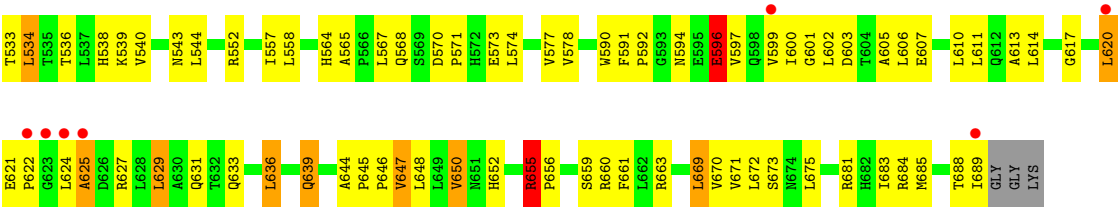
There are 48 discrepancies between the modelled and reference sequences:

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 40.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.80-2.80) 99.6 (40.80-2.80)	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	1863 reflections (4.99%)	wwPDB-VP
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 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -k,-h,-l	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/2727	0.99	12/3703 (0.3%)
1	B	0.54	1/2701 (0.0%)	1.05	17/3671 (0.5%)
All	All	0.52	1/5428 (0.0%)	1.02	29/7374 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	452	GLU	N-CA	5.43	1.53	1.46

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	520	MET	CA-C-N	8.12	128.88	119.47
1	B	520	MET	C-N-CA	8.12	128.88	119.47
1	B	401	LEU	CA-C-N	7.36	125.03	119.66
1	B	401	LEU	C-N-CA	7.36	125.03	119.66
1	B	469	ALA	N-CA-C	6.65	118.53	111.28
1	A	367	VAL	N-CA-C	6.54	118.20	108.46
1	B	402	PRO	N-CA-C	-6.43	104.30	110.47
1	B	596	GLU	N-CA-C	-6.13	102.27	110.55
1	A	433	TYR	CA-C-N	6.05	127.40	119.84
1	A	433	TYR	C-N-CA	6.05	127.40	119.84
1	B	512	LEU	N-CA-C	-6.04	104.78	111.36
1	B	425	VAL	N-CA-C	6.03	117.26	108.58
1	B	498	GLN	N-CA-C	5.57	117.35	111.28
1	B	647	VAL	N-CA-C	5.54	116.28	108.36
1	B	447	GLY	N-CA-C	-5.47	105.29	111.85
1	A	599	VAL	N-CA-C	5.46	116.76	108.80
1	B	650	VAL	N-CA-C	5.42	115.98	108.23
1	A	591	PHE	CA-C-N	5.36	125.28	119.76
1	A	591	PHE	C-N-CA	5.36	125.28	119.76
1	B	451	GLY	N-CA-C	5.31	125.77	113.18
1	B	564	HIS	N-CA-C	5.22	119.75	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	481	VAL	N-CA-C	5.06	115.14	107.75
1	A	564	HIS	N-CA-C	5.04	119.51	112.90
1	A	608	ARG	N-CA-C	-5.04	105.49	111.69
1	B	661	PHE	N-CA-C	5.03	116.62	111.03
1	A	638	ARG	N-CA-C	-5.03	105.69	111.07
1	A	411	MET	N-CA-C	5.02	118.50	112.38
1	A	456	ASP	CA-C-N	5.02	124.62	119.05
1	A	456	ASP	C-N-CA	5.02	124.62	119.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2681	0	2740	220	0
1	B	2655	0	2715	147	0
All	All	5336	0	5455	355	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 33.

All (355) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:511:GLN:HE21	1:B:354:TRP:NE1	1.66	0.93
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:380:ASP:C	1:A:380:ASP:OD1	2.22	0.82
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:HG2	1:B:627:ARG:HH11	1.48	0.79
1:A:376:ASP:HB3	1:A:379:GLN:CG	2.13	0.78
1:A:390:ILE:HD13	1:A:493:ASN:HB2	1.66	0.78
1:B:688:THR:HG22	1:B:689:ILE:H	1.48	0.78
1:A:376:ASP:HB3	1:A:379:GLN:NE2	1.93	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:HD22	1:B:461:LEU:H	1.50	0.76
1:B:472:GLU:HA	1:B:475:GLN:HE21	1.51	0.75
1:B:596:GLU:HG3	1:B:684:ARG:HH11	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
1:A:470:LEU:HD12	1:A:470:LEU:H	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:663:ARG:C	1:A:665:SER:H	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:379:GLN:O	1:A:380:ASP:C	2.34	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:A:367:VAL:HG22	1:A:371:LEU:HB2	1.75	0.68
1:A:397:ASP:C	1:A:398:MET:HE2	2.19	0.68
1:B:621:GLU:CG	1:B:622:PRO:HD2	2.23	0.68
1:A:463:ALA:C	1:A:464:ILE:HD12	2.19	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: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: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:397:ASP:O	1:A:398:MET:HE2	1.97	0.64
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:B:601:GLY:O	1:B:688:THR:HA	1.98	0.63
1:A:470:LEU:H	1:A:470:LEU:CD1	2.13	0.62
1:B:659:SER:O	1:B:663:ARG:HG3	2.00	0.62
1:B:388:ARG:HG2	1:B:388:ARG:HH11	1.63	0.62
1:A:401:LEU:HD11	1:B:352:ALA:HB1	1.82	0.62
1:A:441:ASN:HB2	1:A:479:PHE:HE2	1.63	0.62
1:A:646:PRO:O	1:A:669:LEU:HD12	2.00	0.61
1:B:472:GLU:O	1:B:476:ILE:HG12	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:PRO:O	1:A:379:GLN:NE2	2.34	0.60
1:A:627:ARG:HG3	1:A:627:ARG:HH11	1.66	0.60
1:A:674:ASN:HD22	1:A:675:LEU:HD12	1.66	0.60
1:A:445:ALA:HB2	1:A:478:GLY:HA3	1.83	0.60
1:B:445:ALA:HB3	1:B:478:GLY:O	2.00	0.60
1:B:647:VAL:HG11	1:B:672:LEU:HD22	1.82	0.60
1:B:393:LYS:HE2	1:B:397:ASP:OD2	2.01	0.60
1:B:620:LEU:HD12	1:B:620:LEU:N	2.15	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:445:ALA:CB	1:A:478:GLY:HA3	2.32	0.60
1:A:473:GLN:HA	1:A:476:ILE:HG12	1.83	0.60
1:A:603:ASP:HB3	1:A:606:LEU:HB3	1.82	0.60
1:A:645:PRO:HB2	1:A:647:VAL:HG23	1.84	0.60
1:B:466:ILE:CG2	1:B:470:LEU:HB3	2.32	0.60
1:A:375:VAL:O	1:A:375:VAL:HG13	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:HD2	1:A:453:LYS:N	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:HD12	1:A:470:LEU:N	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
1:B:506:ARG:HA	1:B:538:HIS:CD2	2.41	0.56
1:B:461:LEU:HD22	1:B:461:LEU:N	2.19	0.55
1:B:611:LEU:O	1:B:614:LEU:HB2	2.06	0.55
1:B:639:GLN:NE2	1:B:644:ALA:HB3	2.21	0.55
1:A:350:VAL:HG22	1:A:351:GLU:N	2.20	0.55
1:A:376:ASP:HB3	1:A:379:GLN:CD	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:392:LYS:HZ2	1:B:348:SER:HB3	1.72	0.55
1:A:417:ARG:HG3	1:A:418:TYR:N	2.21	0.54
1:A:502:GLU:OE2	1:A:502:GLU:N	2.34	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:390:ILE:HD12	1:B:493:ASN:HB2	1.90	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:A:674:ASN:HD21	1:A:675:LEU:CD1	2.22	0.53
1:A:375:VAL:HG21	1:A:407:ILE:HG21	1.90	0.53
1:A:376:ASP:CB	1:A:379:GLN:CG	2.84	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:A:370:ARG:HB2	1:A:415:PRO:O	2.08	0.53
1:B:466:ILE:HG23	1:B:470:LEU:HD23	1.90	0.53
1:B:636:LEU:HD13	1:B:636:LEU:O	2.08	0.53
1:A:518:GLN:HG3	1:A:518:GLN:O	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:B:645:PRO:C	1:B:647:VAL:H	2.17	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:B:417:ARG:HH21	1:B:431:ASP:CG	2.18	0.52
1:A:579:ARG:HE	1:A:655:ARG:NH1	2.07	0.52
1:A:600:ILE:HG12	1:A:687:ALA:HB3	1.92	0.52
1:B:534:LEU:HD22	1:B:534:LEU:O	2.10	0.52
1:B:600:ILE:HG13	1:B:639:GLN:OE1	2.09	0.52
1:B:688:THR:CG2	1:B:689:ILE:H	2.18	0.52
1:A:432:ALA:O	1:A:434:PRO:HD3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG22	1:A:689:ILE:O	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: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:600:ILE:HG13	1:A:639:GLN:NE2	2.15	0.51
1:A:474:ALA:O	1:A:479:PHE:HB2	2.11	0.50
1:A:531:VAL:HG12	1:A:565:ALA:CB	2.41	0.50
1:B:438:LEU:HD13	1:B:465:TRP:CE2	2.47	0.50
1:A:603:ASP:HB3	1:A:606:LEU:HB2	1.93	0.50
1:A:684:ARG:O	1:A:686:THR:HG23	2.12	0.50
1:B:440:ILE:HD12	1:B:463:ALA:HB2	1.92	0.50
1:B:655:ARG:HB3	1:B:656:PRO:HD3	1.94	0.50
1:A:392:LYS:HG3	1:B:352:ALA:HB2	1.93	0.50
1:A:638:ARG:O	1:A:642:LEU:HG	2.11	0.50
1:B:600:ILE:HD11	1:B:639:GLN:HG3	1.93	0.50
1:B:463:ALA:C	1:B:464:ILE:HG13	2.35	0.50
1:B:627:ARG:HG2	1:B:627:ARG:NH1	2.23	0.50
1:A:445:ALA:HB2	1:A:478:GLY:C	2.36	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:A:649:LEU:HD23	1:A:677:LEU:HD23	1.94	0.49
1:B:440:ILE:HD13	1:B:456:ASP:HB2	1.94	0.49
1:A:684:ARG:O	1:A:686:THR:N	2.42	0.49
1:A:684:ARG:HD2	1:A:686:THR:HG22	1.94	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:469:ALA:C	1:A:471:LYS:H	2.21	0.48
1:A:600:ILE:CD1	1:A:639:GLN:HG3	2.44	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
1:A:376:ASP:CG	1:A:379:GLN:CG	2.86	0.48
1:A:684:ARG:HD2	1:A:686:THR:CG2	2.44	0.48
1:A:375:VAL:HG22	1:A:407:ILE:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:622:PRO:O	1:A:624:LEU:N	2.47	0.48
1:A:652:HIS:HB2	1:A:675:LEU:HD13	1.96	0.48
1:A:524:THR:O	1:A:527:LEU:N	2.44	0.47
1:A:538:HIS:CE1	1:A:542:GLN:NE2	2.81	0.47
1:A:631:GLN:HG2	1:A:692:LYS:NZ	2.29	0.47
1:A:450:PRO:O	1:A:451:GLY:O	2.32	0.47
1:A:469:ALA:O	1:A:471:LYS:N	2.48	0.47
1:A:473:GLN:HA	1:A:476:ILE:CD1	2.44	0.47
1:B:440:ILE:HG22	1:B:480:THR:O	2.14	0.47
1:B:539:LYS:O	1:B:543:ASN:ND2	2.45	0.47
1:A:370:ARG:NH2	1:A:434:PRO:HD2	2.29	0.47
1:B:507:GLN:HA	1:B:507:GLN:NE2	2.29	0.47
1:B:474:ALA:O	1:B:479:PHE:HB2	2.15	0.47
1:A:591:PHE:CE2	1:A:597:VAL:HG13	2.50	0.47
1:B:461:LEU:H	1:B:461:LEU:CD2	2.23	0.47
1:B:411:MET:HE2	1:B:411:MET:HA	1.96	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:624:LEU:O	1:B:625:ALA:C	2.58	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:596:GLU:CG	1:B:684:ARG:HD3	2.45	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:A:513:LEU:HD23	1:A:537:LEU:HD21	1.97	0.46
1:B:365:MET:HA	1:B:419:ARG:O	2.15	0.46
1:A:645:PRO:HA	1:A:646:PRO:HD3	1.73	0.46
1:B:410:ASN:HD21	1:B:412:ASP:HB2	1.79	0.46
1:B:568:GLN:NE2	1:B:573:GLU:HG3	2.31	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:663:ARG:C	1:A:665:SER:N	2.66	0.46
1:B:596:GLU:H	1:B:596:GLU:CD	2.24	0.46
1:A:645:PRO:C	1:A:647:VAL:H	2.24	0.45
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:528:VAL:HG23	1:A:529:PRO:HA	1.98	0.45
1:A:637:SER:O	1:A:641:MET:HG3	2.17	0.45
1:A:617:GLY:C	1:A:619:GLY:H	2.25	0.45
1:B:444:THR:OG1	1:B:445:ALA:N	2.50	0.45
1:A:533:THR:HG23	1:A:536:THR:H	1.82	0.45
1:A:600:ILE:CG1	1:A:639:GLN:HG3	2.47	0.45
1:A:624:LEU:O	1:A:627:ARG:HB2	2.16	0.45
1:A:631:GLN:O	1:A:632:THR:C	2.60	0.45
1:A:654:LEU:O	1:A:657:LEU:HD23	2.16	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:O	1:A:668:GLN:HG2	2.17	0.44
1:A:376:ASP:CG	1:A:379:GLN:HG2	2.42	0.44
1:A:654:LEU:HB3	1:A:658:LEU:HD12	1.99	0.44
1:A:377:PHE:HD1	1:A:378:GLN:H	1.65	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:B:467:GLU:O	1:B:468:SER:C	2.58	0.44
1:B:536:THR:O	1:B:540:VAL:HG23	2.18	0.44
1:A:367:VAL:CG2	1:A:371:LEU:HB3	2.47	0.44
1:A:369:TYR:HA	1:A:372:ILE:HG13	1.99	0.44
1:A:680:ASN:C	1:A:680:ASN:HD22	2.25	0.44
1:A:394:PHE:HZ	1:A:497:GLY:HA2	1.82	0.44
1:A:418:TYR:CE2	1:A:488:VAL:HG22	2.53	0.44
1:B:363:LEU:HD23	1:B:405:VAL:HG22	1.99	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:A:418:TYR:CD1	1:A:418:TYR:C	2.96	0.43
1:B:645:PRO:HA	1:B:646:PRO:HD3	1.76	0.43
1:B:441:ASN:C	1:B:443:GLY:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:LEU:O	1:B:613:ALA:HB3	2.19	0.43
1:A:371:LEU:HD13	1:A:416:ALA:HA	2.00	0.42
1:A:521:PRO:O	1:A:525:GLU:HG2	2.19	0.42
1:B:567:LEU:O	1:B:567:LEU:HG	2.19	0.42
1:B:646:PRO:O	1:B:669:LEU:HD23	2.18	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: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:B:603:ASP:OD2	1:B:605:ALA:HB3	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:A:547:GLU:O	1:A:548:LYS:HB2	2.17	0.42
1:B:502:GLU:OE1	1:B:502:GLU:N	2.44	0.42
1:B:577:VAL:HG23	1:B:578:VAL:N	2.35	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:361:ASP:O	1:B:423:LYS:HA	2.19	0.42
1:B:620:LEU:HD12	1:B:620:LEU:H	1.82	0.42
1:A:624:LEU:O	1:A:625:ALA:C	2.63	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:HD23	1:A:614:LEU:O	2.19	0.41
1:A:471:LYS:HG3	1:A:481:VAL:HG11	2.02	0.41
1:A:564:HIS:O	1:A:565:ALA:C	2.63	0.41
1:B:366:GLU:HA	1:B:408:ARG:O	2.21	0.41
1:B:377:PHE:HD1	1:B:378:GLN:H	1.62	0.41
1:A:441:ASN:HA	1:A:442:PRO:HD3	1.94	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:B:524:THR:O	1:B:525:GLU:C	2.63	0.41
1:B:536:THR:HG22	1:B:571:PRO:CG	2.47	0.41
1:B:590:TRP:C	1:B:592:PRO:HD3	2.46	0.41
1:B:685:MET:HE3	1:B:688:THR:OG1	2.21	0.41
1:A:351:GLU:HG3	1:A:352:ALA:N	2.36	0.41
1:A:374:MET:O	1:A:381:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:631:GLN:NE2	1:A:692:LYS:HE3	2.36	0.41
1:B:570:ASP:OD2	1:B:570:ASP:C	2.62	0.41
1:B:600:ILE:HG22	1:B:648:LEU:HD13	2.02	0.41
1:A:392:LYS:O	1:A:396:GLN:HG2	2.21	0.41
1:A:464:ILE:HD12	1:A:464:ILE:N	2.36	0.41
1:B:379:GLN:HE21	1:B:379:GLN:HB3	1.62	0.41
1:B:531:VAL:HG12	1:B:565:ALA:CB	2.51	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:HE21	1:A:668:GLN:HB3	1.58	0.40
1:A:441:ASN:C	1:A:441:ASN:HD22	2.29	0.40
1:A:359:LEU:N	1:A:359:LEU:CD1	2.85	0.40
1:A:370:ARG:HH21	1:A:434:PRO:HD2	1.86	0.40
1:A:444:THR:OG1	1:A:445:ALA:N	2.42	0.40
1:A:631:GLN:O	1:A:634:GLU:N	2.52	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%)	1	3
1	B	340/389 (87%)	296 (87%)	33 (10%)	11 (3%)	3	11
All	All	684/778 (88%)	590 (86%)	62 (9%)	32 (5%)	2	6

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	445	ALA

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Mol	Chain	Res	Type
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
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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/328 (88%)	256 (89%)	33 (11%)	5	19
1	B	287/328 (88%)	266 (93%)	21 (7%)	13	38
All	All	576/656 (88%)	522 (91%)	54 (9%)	8	27

All (54) 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	404	VAL
1	A	409	ASP
1	A	413	LEU
1	A	421	LEU
1	A	436	ARG
1	A	440	ILE
1	A	470	LEU
1	A	500	SER
1	A	503	LEU
1	A	510	GLN
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	611	LEU
1	A	620	LEU
1	A	649	LEU
1	A	655	ARG
1	A	674	ASN
1	A	677	LEU
1	A	679	ASP

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Mol	Chain	Res	Type
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	404	VAL
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
1	B	620	LEU
1	B	636	LEU
1	B	639	GLN
1	B	650	VAL
1	B	655	ARG
1	B	669	LEU

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	379	GLN
1	A	414	GLN
1	A	441	ASN
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	631	GLN
1	A	668	GLN
1	A	674	ASN
1	A	680	ASN
1	B	358	GLN
1	B	378	GLN
1	B	379	GLN

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Mol	Chain	Res	Type
1	B	410	ASN
1	B	475	GLN
1	B	477	GLN
1	B	498	GLN
1	B	538	HIS
1	B	572	HIS
1	B	615	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	346/389 (88%)	0.50	29 (8%) 17 12	37, 74, 123, 137	0
1	B	342/389 (87%)	0.37	17 (4%) 34 26	33, 72, 114, 130	0
All	All	688/778 (88%)	0.43	46 (6%) 24 17	33, 73, 122, 137	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	379	GLN	4.9
1	A	620	LEU	4.8
1	B	620	LEU	4.8
1	A	380	ASP	4.4
1	B	446	ALA	3.9
1	B	622	PRO	3.6
1	A	377	PHE	3.4
1	A	622	PRO	3.1
1	B	377	PHE	3.0
1	B	349	VAL	3.0
1	A	625	ALA	2.9
1	A	470	LEU	2.8
1	A	689	ILE	2.8
1	A	649	LEU	2.7
1	B	449	LEU	2.7
1	A	607	GLU	2.6
1	B	624	LEU	2.6
1	B	479	PHE	2.5
1	B	451	GLY	2.5
1	A	685	MET	2.5
1	B	689	ILE	2.5
1	B	459	PHE	2.5
1	A	623	GLY	2.4
1	A	469	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	450	PRO	2.4
1	A	594	ASN	2.3
1	A	381	GLY	2.3
1	B	625	ALA	2.3
1	A	668	GLN	2.3
1	A	692	LYS	2.3
1	A	476	ILE	2.3
1	A	520	MET	2.2
1	A	661	PHE	2.2
1	A	691	GLY	2.2
1	B	447	GLY	2.2
1	A	526	ASP	2.2
1	B	623	GLY	2.1
1	A	602	LEU	2.1
1	B	466	ILE	2.1
1	A	442	PRO	2.1
1	A	523	LEU	2.1
1	A	449	LEU	2.0
1	A	609	LEU	2.0
1	B	448	THR	2.0
1	B	599	VAL	2.0
1	A	479	PHE	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.