



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2026 – 01:51 AM UTC

PDB ID : 2AKA / pdb_00002aka
Title : Structure of the nucleotide-free myosin II motor domain from Dictyostelium discoideum fused to the GTPase domain of dynamin 1 from Rattus norvegicus
Authors : Reubold, T.F.; Eschenburg, S.; Becker, A.; Leonard, M.; Schmid, S.L.; Vallee, R.B.; Kull, F.J.; Manstein, D.J.
Deposited on : 2005-08-03
Resolution : 1.90 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

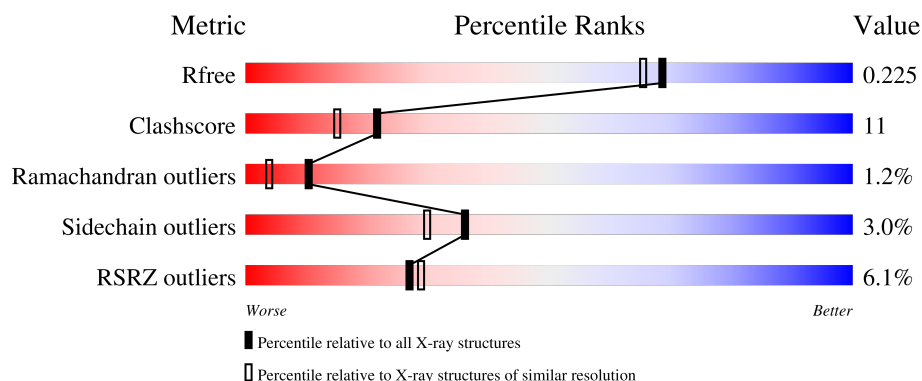
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	776	6% 79% 17% ..
2	L	13	8% 31% 15% 54%
3	B	299	5% 76% 20% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9377 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 myosin II heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	764	Total	C	N	O	S	0	20	0
			6227	3948	1081	1182	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	insertion	UNP P08799
A	-9	HIS	-	insertion	UNP P08799
A	-8	HIS	-	insertion	UNP P08799
A	-7	HIS	-	insertion	UNP P08799
A	-6	HIS	-	insertion	UNP P08799
A	-5	HIS	-	insertion	UNP P08799
A	-4	HIS	-	insertion	UNP P08799
A	-3	HIS	-	insertion	UNP P08799
A	-2	ASP	-	insertion	UNP P08799
A	-1	GLY	-	insertion	UNP P08799
A	0	THR	-	insertion	UNP P08799
A	1	GLU	-	insertion	UNP P08799

- Molecule 2 is a protein called LINKER.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	L	6	Total	C	N	O	0	0	0
			51	32	12	7			

- Molecule 3 is a protein called Dynamin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	299	Total	C	N	O	S	0	3	0
			2345	1474	420	442	9			

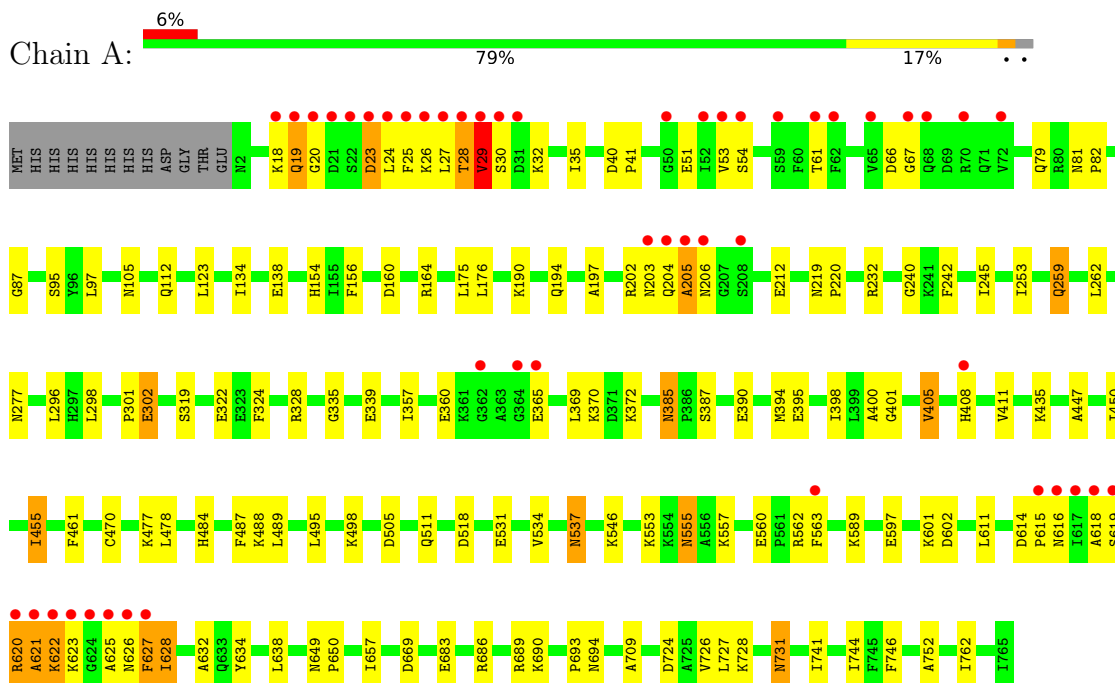
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	584	Total 584	O 584	0	0
4	B	170	Total 170	O 170	0	0

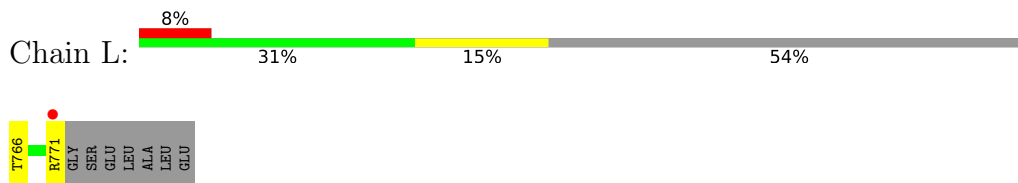
3 Residue-property plots [i](#)

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.

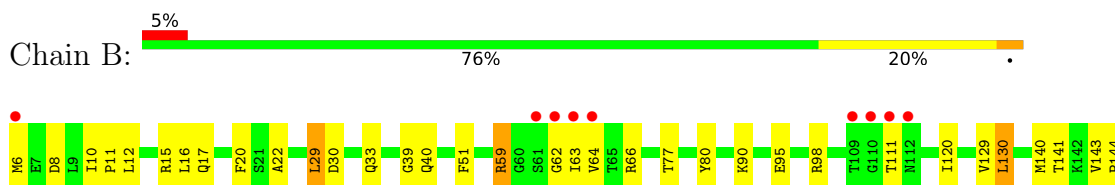
- Molecule 1: myosin II heavy chain

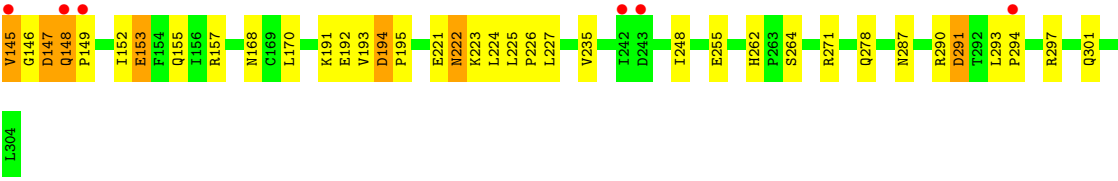


- Molecule 2: LINKER



- Molecule 3: Dynamin-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.42Å 126.99Å 160.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 1.90 19.93 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.93-1.90) 99.1 (19.93-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.81 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.185 , 0.224 0.187 , 0.225	Depositor DCC
R_{free} test set	2317 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.2	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	0.96	EDS
Total number of atoms	9377	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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	0.93	0/6427	1.07	23/8670 (0.3%)
2	L	0.80	0/51	0.93	0/68
3	B	0.83	0/2393	1.10	10/3238 (0.3%)
All	All	0.90	0/8871	1.08	33/11976 (0.3%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	563	PHE	N-CA-C	9.24	122.20	109.54
1	A	203	ASN	N-CA-C	7.85	122.67	113.18
1	A	262	LEU	N-CA-C	7.37	121.57	111.39
1	A	245	ILE	N-CA-C	-7.31	97.05	108.23
1	A	560	GLU	N-CA-C	-7.13	99.33	109.24
1	A	447	ALA	N-CA-C	-6.99	104.38	113.12
1	A	202	ARG	N-CA-C	-6.65	102.46	110.44
1	A	81	ASN	CA-C-N	6.61	126.59	119.78
1	A	81	ASN	C-N-CA	6.61	126.59	119.78
3	B	51	PHE	N-CA-C	-6.58	104.03	111.14
1	A	335	GLY	N-CA-C	6.53	124.63	115.43
1	A	411	VAL	N-CA-C	6.37	117.12	110.62
1	A	534	VAL	N-CA-C	6.19	117.20	111.45
1	A	277	ASN	N-CA-C	-6.15	102.56	110.19
3	B	225	LEU	CA-C-N	5.99	127.33	119.84
3	B	225	LEU	C-N-CA	5.99	127.33	119.84
3	B	130	LEU	N-CA-C	-5.89	101.75	110.46
1	A	649	ASN	N-CA-C	-5.80	100.23	109.04
1	A	511	GLN	N-CA-C	5.68	117.47	111.28
3	B	120	ILE	N-CA-C	-5.65	100.26	108.17
1	A	562	ARG	CA-C-N	-5.59	114.83	122.87
1	A	562	ARG	C-N-CA	-5.59	114.83	122.87
1	A	123	LEU	N-CA-C	-5.47	99.81	108.73
1	A	450	ILE	N-CA-C	-5.46	98.07	107.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	GLY	N-CA-C	-5.41	100.35	113.18
3	B	248	ILE	N-CA-C	5.39	116.12	110.62
1	A	669	ASP	N-CA-C	5.38	117.14	111.28
3	B	194	ASP	CA-C-N	5.37	125.44	119.32
3	B	194	ASP	C-N-CA	5.37	125.44	119.32
3	B	291	ASP	N-CA-C	5.23	117.06	111.36
1	A	693	PRO	N-CA-C	5.21	120.78	113.53
1	A	657	ILE	N-CA-C	-5.11	104.24	108.63
3	B	39	GLY	N-CA-C	-5.08	105.59	112.14

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	6227	0	6170	138	0
2	L	51	0	59	4	0
3	B	2345	0	2402	49	0
4	A	584	0	0	9	0
4	B	170	0	0	3	0
All	All	9377	0	8631	187	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 11.

All (187) 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:154:HIS:HD2	1:A:156:PHE:H	1.12	0.97
3:B:40:GLN:NE2	3:B:141:THR:HG21	1.85	0.91
3:B:40:GLN:HB2	3:B:141:THR:HG22	1.57	0.84
1:A:589:LYS:HD3	4:A:1018:HOH:O	1.79	0.82
1:A:154:HIS:CD2	1:A:156:PHE:H	1.98	0.81
1:A:498:LYS:HD3	1:A:741:ILE:HD11	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:LYS:C	1:A:625:ALA:H	1.90	0.79
1:A:197:ALA:HA	1:A:253:ILE:HD12	1.64	0.78
3:B:222:ASN:HD21	3:B:227:LEU:H	1.30	0.78
1:A:628:ILE:H	1:A:628:ILE:HD12	1.49	0.77
2:L:766:THR:HG21	3:B:301:GLN:HG2	1.68	0.76
1:A:686[B]:ARG:HH11	1:A:686[B]:ARG:HB3	1.51	0.76
3:B:12:LEU:HA	3:B:15:ARG:NH1	2.01	0.75
1:A:35:ILE:HD13	1:A:79:GLN:HA	1.69	0.74
3:B:6:MET:HG3	3:B:8:ASP:H	1.54	0.73
1:A:301:PRO:HG2	1:A:302[A]:GLU:OE1	1.89	0.72
1:A:19:GLN:O	1:A:23:ASP:HB3	1.90	0.71
1:A:484:HIS:HE1	1:A:488:LYS:NZ	1.88	0.71
1:A:628:ILE:HD12	1:A:628:ILE:N	2.07	0.69
3:B:63:ILE:HD13	3:B:66:ARG:HG2	1.72	0.69
1:A:686[B]:ARG:HB3	1:A:686[B]:ARG:NH1	2.08	0.69
1:A:190:LYS:HZ2	1:A:194:GLN:NE2	1.91	0.68
1:A:87:GLY:H	1:A:105:ASN:ND2	1.92	0.68
1:A:28:THR:O	1:A:29:VAL:HG22	1.93	0.67
1:A:531:GLU:OE1	1:A:546:LYS:NZ	2.27	0.67
1:A:232[A]:ARG:HG3	1:A:461:PHE:CE1	2.32	0.65
1:A:240:GLY:HA3	1:A:455:ILE:HG23	1.79	0.64
3:B:17:GLN:HE21	3:B:33:GLN:HE21	1.44	0.64
1:A:537:ASN:H	1:A:537:ASN:HD22	1.45	0.64
1:A:18:LYS:HG2	1:A:112:GLN:OE1	1.97	0.64
3:B:40:GLN:CD	3:B:62:GLY:HA2	2.22	0.63
1:A:23:ASP:OD2	1:A:24:LEU:HG	1.98	0.63
1:A:628:ILE:HG22	1:A:632:ALA:HB3	1.79	0.63
1:A:54:SER:HB3	1:A:61:THR:HB	1.81	0.62
3:B:143:VAL:O	3:B:145:VAL:HG12	1.99	0.61
1:A:339:GLU:HG3	4:A:964:HOH:O	1.99	0.61
3:B:40:GLN:CD	3:B:141:THR:HG21	2.24	0.61
1:A:95:SER:HA	1:A:694:ASN:HD21	1.66	0.60
3:B:293:LEU:N	3:B:294:PRO:HD2	2.16	0.60
1:A:240:GLY:HA3	1:A:455:ILE:CG2	2.32	0.59
1:A:623:LYS:C	1:A:625:ALA:N	2.56	0.59
1:A:555:ASN:HD22	1:A:557:LYS:H	1.51	0.59
1:A:35:ILE:CD1	1:A:79:GLN:HG2	2.31	0.59
1:A:19:GLN:HG3	1:A:20:GLY:H	1.66	0.59
1:A:622:LYS:O	1:A:628:ILE:HD11	2.02	0.58
1:A:19:GLN:HB3	1:A:24:LEU:HB2	1.85	0.58
1:A:689:ARG:NH2	4:A:871:HOH:O	2.26	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:ASN:ND2	1:A:557:LYS:H	2.02	0.58
1:A:19:GLN:HG3	1:A:20:GLY:N	2.20	0.57
1:A:53:VAL:CG2	1:A:61:THR:HG22	2.34	0.57
1:A:35:ILE:HD11	1:A:79:GLN:HG2	1.86	0.57
1:A:232[A]:ARG:HG3	1:A:461:PHE:HE1	1.67	0.57
1:A:395:GLU:HG2	1:A:408:HIS:ND1	2.20	0.57
1:A:385:ASN:HD22	1:A:385:ASN:C	2.13	0.56
1:A:372:LYS:HE3	1:A:390:GLU:OE2	2.05	0.56
1:A:190:LYS:NZ	1:A:194:GLN:NE2	2.52	0.56
2:L:766:THR:CG2	3:B:301:GLN:HG2	2.34	0.56
1:A:484:HIS:CE1	1:A:488:LYS:HE3	2.40	0.56
1:A:242:PHE:HB3	1:A:259:GLN:HG2	1.87	0.55
3:B:12:LEU:HA	3:B:15:ARG:HH12	1.70	0.54
1:A:53:VAL:HG23	1:A:54:SER:N	2.22	0.54
1:A:435:LYS:NZ	4:A:1041:HOH:O	2.40	0.54
1:A:398:ILE:C	1:A:398:ILE:HD12	2.34	0.53
1:A:23:ASP:O	1:A:27:LEU:HD13	2.08	0.53
1:A:470:CYS:HB3	1:A:634:TYR:CZ	2.43	0.53
3:B:40:GLN:HB2	3:B:141:THR:CG2	2.33	0.53
1:A:628:ILE:H	1:A:628:ILE:CD1	2.19	0.53
1:A:319:SER:OG	1:A:322:GLU:HG3	2.09	0.53
1:A:620:ARG:HH21	1:A:628:ILE:HD13	1.73	0.52
1:A:53:VAL:HG22	1:A:61:THR:O	2.09	0.52
1:A:385:ASN:ND2	1:A:387:SER:H	2.07	0.52
1:A:683:GLU:OE2	1:A:686[B]:ARG:NH1	2.42	0.52
1:A:484:HIS:CE1	1:A:488:LYS:CE	2.93	0.52
3:B:262:HIS:CE1	3:B:264:SER:HB2	2.45	0.52
3:B:221:GLU:O	3:B:223:LYS:HE2	2.10	0.52
1:A:19:GLN:CB	1:A:24:LEU:HB2	2.39	0.52
3:B:271:ARG:HH11	3:B:271:ARG:HG3	1.75	0.52
1:A:614:ASP:OD1	1:A:616:ASN:HB2	2.10	0.52
3:B:149:PRO:HG2	3:B:155:GLN:HE22	1.75	0.52
1:A:204:GLN:O	1:A:205:ALA:HB3	2.08	0.52
1:A:744:ILE:HD13	1:A:746:PHE:CZ	2.45	0.52
1:A:190:LYS:HZ2	1:A:194:GLN:HE22	1.58	0.51
1:A:97:LEU:O	1:A:689:ARG:HD2	2.10	0.51
1:A:498:LYS:HD3	1:A:741:ILE:CD1	2.39	0.51
1:A:197:ALA:HA	1:A:253:ILE:CD1	2.36	0.51
1:A:204:GLN:O	1:A:205:ALA:CB	2.58	0.51
1:A:619:SER:O	1:A:620:ARG:CB	2.59	0.50
1:A:28:THR:HG22	1:A:29:VAL:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:771:ARG:HD3	3:B:297:ARG:HD3	1.94	0.50
1:A:357:ILE:HG23	1:A:369:LEU:HD11	1.94	0.50
1:A:477:LYS:HG3	1:A:638:LEU:HD21	1.94	0.50
1:A:296:LEU:HB2	1:A:298:LEU:HG	1.93	0.49
3:B:59:ARG:NE	4:B:447:HOH:O	2.46	0.49
1:A:95:SER:HB3	1:A:752:ALA:HB2	1.94	0.48
1:A:204:GLN:OE1	1:A:204:GLN:HA	2.12	0.48
3:B:287:ASN:ND2	3:B:290:ARG:HH12	2.10	0.48
1:A:601:LYS:HE2	4:A:1232:HOH:O	2.13	0.48
3:B:147:ASP:O	3:B:148:GLN:CB	2.60	0.48
3:B:157[A]:ARG:NH2	3:B:192:GLU:OE2	2.39	0.48
3:B:40:GLN:NE2	3:B:62:GLY:HA2	2.28	0.48
3:B:40:GLN:CB	3:B:141:THR:HG22	2.38	0.48
1:A:484:HIS:CE1	1:A:488:LYS:NZ	2.77	0.47
1:A:683:GLU:CD	1:A:686[B]:ARG:HH12	2.21	0.47
3:B:271:ARG:HG3	3:B:271:ARG:NH1	2.30	0.47
1:A:400:ALA:HB2	1:A:405:VAL:HG11	1.97	0.47
3:B:30:ASP:OD1	3:B:168:ASN:HB2	2.13	0.47
3:B:193:VAL:C	3:B:195:PRO:HD3	2.39	0.47
1:A:611:LEU:O	1:A:618:ALA:HB2	2.15	0.47
3:B:22:ALA:HB3	4:B:430:HOH:O	2.15	0.47
1:A:727:LEU:HD11	1:A:744:ILE:CD1	2.45	0.47
1:A:455:ILE:HD11	1:A:478:LEU:CD1	2.45	0.46
1:A:484:HIS:HE1	1:A:488:LYS:CE	2.28	0.46
1:A:683:GLU:CD	1:A:686[B]:ARG:NH1	2.73	0.46
1:A:762:ILE:O	2:L:766:THR:HG23	2.15	0.46
3:B:10:ILE:HB	3:B:11:PRO:HD3	1.97	0.46
1:A:160:ASP:O	1:A:164:ARG:HG2	2.14	0.46
1:A:518:ASP:OD1	1:A:518:ASP:C	2.57	0.46
3:B:129:VAL:HA	3:B:278:GLN:HE22	1.80	0.46
1:A:621:ALA:O	1:A:622:LYS:HG3	2.14	0.46
1:A:724:ASP:OD2	1:A:728:LYS:HE3	2.16	0.46
1:A:623:LYS:HG2	1:A:623:LYS:O	2.16	0.46
3:B:140:MET:O	3:B:141:THR:HG22	2.15	0.46
1:A:385:ASN:HD22	1:A:387:SER:H	1.63	0.46
1:A:53:VAL:HG23	1:A:54:SER:H	1.80	0.45
1:A:194:GLN:HG2	1:A:212:GLU:OE1	2.16	0.45
1:A:18:LYS:O	1:A:19:GLN:C	2.59	0.45
1:A:470:CYS:HB3	1:A:634:TYR:CE2	2.51	0.45
3:B:235:VAL:HG22	3:B:255:GLU:HG3	1.99	0.45
3:B:143:VAL:C	3:B:145:VAL:H	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:144:PRO:O	3:B:146:GLY:N	2.50	0.45
1:A:484:HIS:HE1	1:A:488:LYS:HZ1	1.65	0.45
1:A:385:ASN:HD22	1:A:387:SER:N	2.15	0.44
3:B:143:VAL:HA	3:B:144:PRO:HD2	1.83	0.44
1:A:30:SER:OG	1:A:32:LYS:NZ	2.44	0.44
3:B:80:TYR:CD1	3:B:90:LYS:HD2	2.53	0.44
3:B:194:ASP:N	3:B:195:PRO:HD3	2.33	0.44
1:A:537:ASN:H	1:A:537:ASN:ND2	2.13	0.44
1:A:324:PHE:CE2	1:A:328[B]:ARG:HD2	2.53	0.44
1:A:626:ASN:OD1	1:A:627:PHE:N	2.50	0.44
1:A:690:LYS:HE2	4:A:917:HOH:O	2.18	0.43
1:A:620:ARG:O	1:A:621:ALA:HB2	2.17	0.43
3:B:130:LEU:H	3:B:278:GLN:NE2	2.16	0.43
1:A:495:LEU:HD23	1:A:495:LEU:HA	1.91	0.43
1:A:686[B]:ARG:HH11	1:A:686[B]:ARG:CB	2.27	0.43
1:A:26:LYS:O	1:A:26:LYS:HG3	2.19	0.43
1:A:32:LYS:HD2	1:A:51:GLU:OE1	2.19	0.43
1:A:369:LEU:HD12	1:A:369:LEU:HA	1.84	0.43
1:A:175:LEU:C	1:A:175:LEU:HD23	2.44	0.43
1:A:176:LEU:HD12	1:A:176:LEU:N	2.34	0.43
1:A:324:PHE:O	1:A:328[A]:ARG:HG3	2.19	0.43
3:B:152:ILE:HG23	3:B:153:GLU:N	2.34	0.42
1:A:242:PHE:HB3	1:A:259:GLN:CG	2.48	0.42
1:A:709:ALA:HB2	1:A:726:VAL:HA	2.01	0.42
1:A:328[B]:ARG:NH2	4:A:1198:HOH:O	2.25	0.42
3:B:95:GLU:OE1	3:B:98[A]:ARG:NH2	2.42	0.42
3:B:191:LYS:NZ	4:B:382:HOH:O	2.52	0.42
1:A:627:PHE:CD1	1:A:628:ILE:O	2.72	0.42
1:A:27:LEU:O	1:A:28:THR:HB	2.20	0.42
3:B:63:ILE:CD1	3:B:66:ARG:HG2	2.46	0.41
1:A:487:PHE:CD1	1:A:505:ASP:HA	2.55	0.41
1:A:622:LYS:HB3	1:A:623:LYS:H	1.59	0.41
3:B:29:LEU:HD12	3:B:29:LEU:HA	1.90	0.41
1:A:219[B]:ASN:HB2	1:A:220:PRO:CD	2.49	0.41
1:A:328[B]:ARG:NE	4:A:1198:HOH:O	2.45	0.41
1:A:619:SER:O	1:A:620:ARG:HB3	2.19	0.41
3:B:16:LEU:O	3:B:20:PHE:HD1	2.03	0.41
3:B:145:VAL:O	3:B:145:VAL:HG13	2.19	0.41
1:A:35:ILE:HD13	1:A:79:GLN:HG2	2.02	0.41
1:A:489:LEU:HD23	1:A:489:LEU:HA	1.80	0.41
1:A:134:ILE:O	1:A:154:HIS:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219[A]:ASN:HB3	1:A:220:PRO:HD3	2.03	0.41
1:A:487:PHE:CG	1:A:505:ASP:HA	2.56	0.41
1:A:40:ASP:HA	1:A:41:PRO:HD2	1.92	0.41
1:A:360:GLU:OE1	1:A:370:LYS:HD2	2.21	0.41
1:A:623:LYS:O	1:A:625:ALA:N	2.53	0.41
1:A:19:GLN:HA	1:A:24:LEU:HG	2.03	0.41
1:A:240:GLY:CA	1:A:455:ILE:CG2	2.98	0.41
3:B:224:LEU:C	3:B:226:PRO:HD3	2.45	0.41
1:A:219[B]:ASN:HB2	1:A:220:PRO:HD3	2.03	0.41
1:A:390:GLU:HG2	1:A:394:MET:CE	2.50	0.41
1:A:555:ASN:HD22	1:A:557:LYS:N	2.16	0.40
1:A:614:ASP:HA	1:A:615:PRO:HD2	1.84	0.40
3:B:17:GLN:HE21	3:B:33:GLN:NE2	2.16	0.40
1:A:219[A]:ASN:ND2	4:A:1327:HOH:O	2.54	0.40
1:A:597:GLU:O	1:A:601:LYS:HG3	2.22	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	782/776 (101%)	744 (95%)	28 (4%)	10 (1%)	9	3
2	L	4/13 (31%)	4 (100%)	0	0	100	100
3	B	300/299 (100%)	283 (94%)	14 (5%)	3 (1%)	12	5
All	All	1086/1088 (100%)	1031 (95%)	42 (4%)	13 (1%)	10	4

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	205	ALA

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Mol	Chain	Res	Type
1	A	620	ARG
1	A	621	ALA
1	A	622	LYS
3	B	145	VAL
1	A	28	THR
1	A	29	VAL
1	A	25	PHE
1	A	19	GLN
3	B	147	ASP
3	B	148	GLN
1	A	67	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	688/679 (101%)	666 (97%)	22 (3%)	34	27
2	L	6/11 (54%)	6 (100%)	0	100	100
3	B	263/261 (101%)	254 (97%)	9 (3%)	32	25
All	All	957/951 (101%)	926 (97%)	31 (3%)	36	27

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	66	ASP
1	A	82	PRO
1	A	138	GLU
1	A	206	ASN
1	A	259	GLN
1	A	302[A]	GLU
1	A	302[B]	GLU
1	A	365	GLU
1	A	385	ASN
1	A	405	VAL

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Mol	Chain	Res	Type
1	A	455	ILE
1	A	537	ASN
1	A	553	LYS
1	A	555	ASN
1	A	602[A]	ASP
1	A	602[B]	ASP
1	A	627	PHE
1	A	628	ILE
1	A	650	PRO
1	A	731[A]	ASN
1	A	731[B]	ASN
3	B	29	LEU
3	B	59	ARG
3	B	64	VAL
3	B	77	THR
3	B	111	THR
3	B	153	GLU
3	B	170	LEU
3	B	222	ASN
3	B	291	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	12	HIS
1	A	105	ASN
1	A	154	HIS
1	A	188	ASN
1	A	194	GLN
1	A	234	ASN
1	A	259	GLN
1	A	305	ASN
1	A	329	GLN
1	A	385	ASN
1	A	407	GLN
1	A	439	ASN
1	A	443	GLN
1	A	484	HIS
1	A	485	HIS
1	A	491	GLN
1	A	500	ASN

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Mol	Chain	Res	Type
1	A	537	ASN
1	A	555	ASN
1	A	613	ASN
1	A	616	ASN
1	A	694	ASN
1	A	711	ASN
1	A	729	HIS
1	A	760	GLN
3	B	25	GLN
3	B	33	GLN
3	B	40	GLN
3	B	121	ASN
3	B	128	HIS
3	B	155	GLN
3	B	222	ASN
3	B	278	GLN
3	B	283	GLN
3	B	287	ASN

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 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 ⓘ

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	764/776 (98%)	0.01	49 (6%) 25 27	10, 25, 64, 102	20 (2%)
2	L	6/13 (46%)	0.99	1 (16%) 4 4	40, 46, 53, 66	0
3	B	299/299 (100%)	0.13	15 (5%) 34 36	18, 30, 63, 76	3 (1%)
All	All	1069/1088 (98%)	0.05	65 (6%) 27 29	10, 26, 64, 102	23 (2%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	29	VAL	7.6
1	A	25	PHE	6.3
1	A	20	GLY	6.1
1	A	621	ALA	5.8
1	A	625	ALA	5.7
1	A	24	LEU	5.4
1	A	27	LEU	5.3
1	A	618	ALA	5.2
1	A	623	LYS	4.7
1	A	28	THR	4.7
1	A	624	GLY	4.6
1	A	365	GLU	4.5
1	A	626	ASN	4.5
1	A	206	ASN	4.5
1	A	617	ILE	4.5
1	A	31	ASP	4.2
1	A	619	SER	3.9
1	A	622	LYS	3.9
3	B	242	ILE	3.9
3	B	110	GLY	3.8
1	A	620	ARG	3.7
1	A	72	VAL	3.7
1	A	62	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	22	SER	3.6
1	A	23	ASP	3.5
1	A	19	GLN	3.5
1	A	627	PHE	3.4
1	A	30	SER	3.3
1	A	52	ILE	3.2
3	B	145	VAL	3.2
1	A	26	LYS	3.1
1	A	204	GLN	3.1
3	B	6	MET	3.0
3	B	61	SER	2.9
3	B	148	GLN	2.8
1	A	203	ASN	2.8
1	A	61	THR	2.8
3	B	111	THR	2.8
1	A	53	VAL	2.7
3	B	112	ASN	2.7
1	A	205	ALA	2.7
1	A	563	PHE	2.6
1	A	50	GLY	2.6
1	A	208	SER	2.5
1	A	65	VAL	2.5
3	B	149	PRO	2.5
1	A	408	HIS	2.3
1	A	616	ASN	2.3
3	B	294	PRO	2.3
3	B	243	ASP	2.3
2	L	771	ARG	2.3
1	A	362	GLY	2.3
3	B	64	VAL	2.2
1	A	21	ASP	2.2
1	A	59	SER	2.2
1	A	67	GLY	2.2
1	A	68	GLN	2.1
1	A	54	SER	2.1
1	A	18	LYS	2.1
1	A	615	PRO	2.1
3	B	109	THR	2.0
1	A	364	GLY	2.0
1	A	70	ARG	2.0
3	B	63	ILE	2.0
3	B	62	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 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.