Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:00 am BST

PDB ID	:	2AKA
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 following versions of software and data (see references ⓘ) were used in the production of this report:

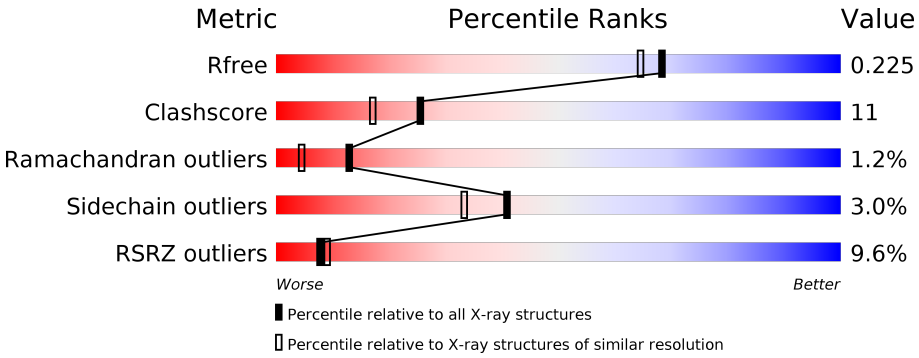
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	776	9% 81% 15%
2	L	13	15% 31% 15% 54%
3	B	299	11% 79% 19%

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			

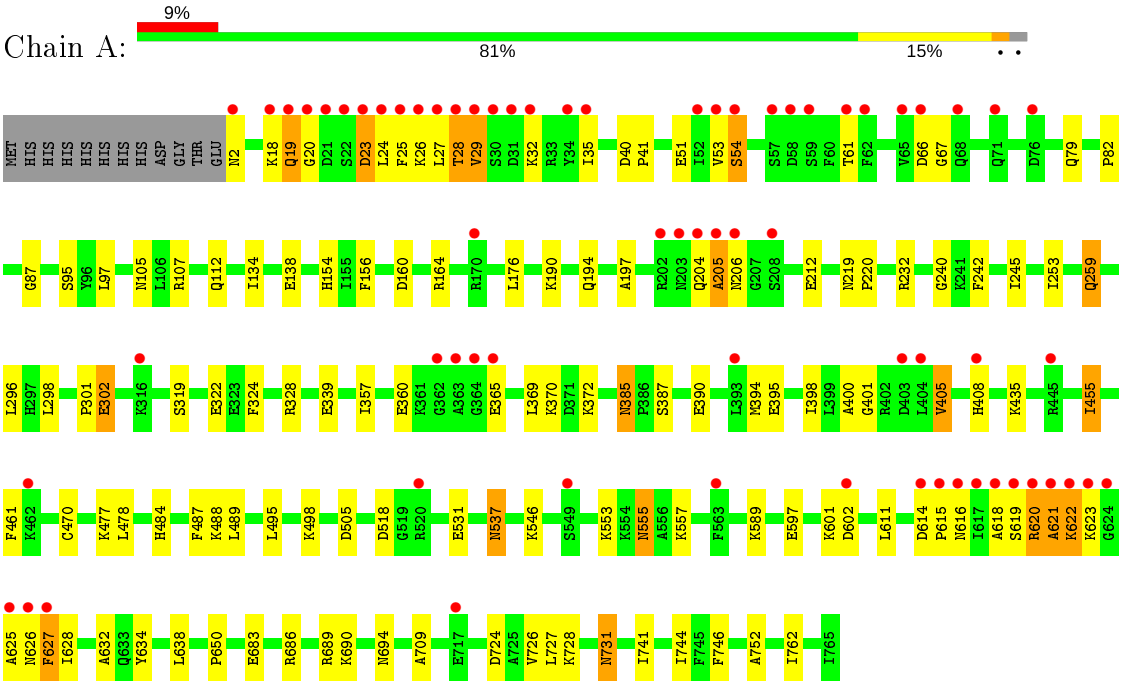
- Molecule 4 is water.

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

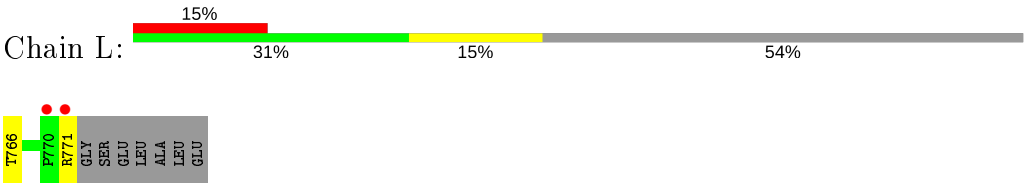
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

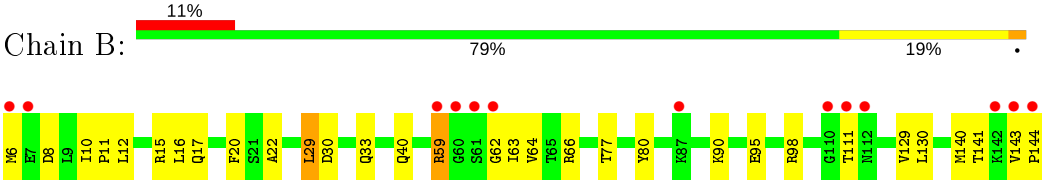
- Molecule 1: myosin II heavy chain

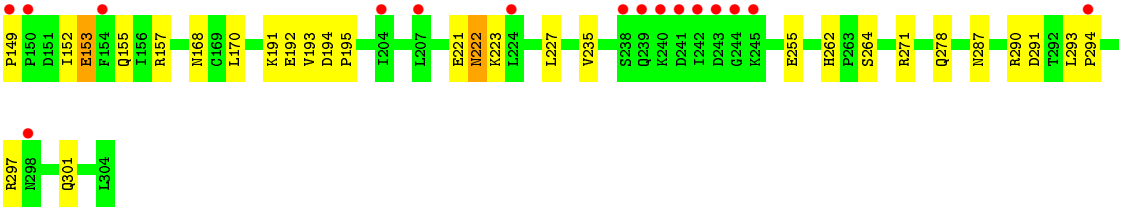


- Molecule 2: LINKER



- Molecule 3: Dynamin-1




P149
P150
D151
I152
E153
F154
Q155
I156
R157
N168
C169
L170
K191
E192
V193
D194
P195
I204
L207
E221
N222
K223
L224
L227
V235
S238
Q239
K240
D241
I242
D243
G244
K245
E255
H262
P263
S264
R271
Q278
N287
R290
D291
T292
L293
P294
R297
M298
Q301
L304

4 Data and refinement statistics (i)

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) 99.3 (19.93-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [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)	0.37 , 54.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.81	0/6427	0.80	3/8670 (0.0%)
2	L	0.53	0/51	0.61	0/68
3	B	0.69	0/2393	0.81	0/3238
All	All	0.78	0/8871	0.80	3/11976 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	107	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	A	245	ILE	N-CA-C	-5.17	97.05	111.00
1	A	401	GLY	N-CA-C	-5.10	100.35	113.10

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	136	0
2	L	51	0	59	4	0
3	B	2345	0	2402	48	0
4	A	584	0	0	9	0
4	B	170	0	0	3	0
All	All	9377	0	8631	184	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 (184) 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
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:HD12	1:A:628:ILE:H	1.49	0.77
2:L:766:THR:HG21	3:B:301:GLN:HG2	1.68	0.76
1:A:686[B]:ARG:HB3	1:A:686[B]:ARG:HH11	1.51	0.76
3:B:12:LEU:HA	3:B:15:ARG:NH1	2.01	0.75
1:A:623:LYS:C	1:A:625:ALA:H	1.90	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:HD22	1:A:537:ASN:H	1.45	0.64
1:A:18:LYS:HG2	1:A:112:GLN:OE1	1.97	0.64
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:GLY:HA3	1:A:455:ILE:CG2	2.32	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:623:LYS:C	1:A:625:ALA:N	2.56	0.59
1:A:19:GLN:HG3	1:A:20:GLY:H	1.66	0.59
3:B:40:GLN:CD	3:B:62:GLY:HA2	2.22	0.58
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
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:232[A]:ARG:HG3	1:A:461:PHE:HE1	1.67	0.57
1:A:35:ILE:HD11	1:A:79:GLN:HG2	1.86	0.57
1:A:395:GLU:HG2	1:A:408:HIS:ND1	2.20	0.57
1:A:372:LYS:HE3	1:A:390:GLU:OE2	2.05	0.56
2:L:766:THR:CG2	3:B:301:GLN:HG2	2.34	0.56
1:A:190:LYS:NZ	1:A:194:GLN:NE2	2.52	0.56
3:B:40:GLN:CD	3:B:141:THR:HG21	2.24	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: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:CD1	1:A:628:ILE:H	2.19	0.53
1:A:204:GLN:O	1:A:205:ALA:HB3	2.08	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:385:ASN:ND2	1:A:387:SER:H	2.07	0.52
1:A:53:VAL:HG22	1:A:61:THR:O	2.09	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
1:A:385:ASN:C	1:A:385:ASN:HD22	2.13	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:HG3	3:B:271:ARG:HH11	1.75	0.52
1:A:614:ASP:OD1	1:A:616:ASN:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:149:PRO:HG2	3:B:155:GLN:HE22	1.75	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:28:THR:HG22	1:A:29:VAL:N	2.25	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
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:398:ILE:HD12	1:A:398:ILE:C	2.34	0.49
1:A:204:GLN:HA	1:A:204:GLN:OE1	2.12	0.48
1:A:95:SER:HB3	1:A:752:ALA:HB2	1.94	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:CB	3:B:141:THR:HG22	2.38	0.48
3:B:40:GLN:NE2	3:B:62:GLY:HA2	2.28	0.48
1:A:484:HIS:CE1	1:A:488:LYS:NZ	2.77	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
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
3:B:10:ILE:HB	3:B:11:PRO:HD3	1.97	0.46
1:A:762:ILE:O	2:L:766:THR:HG23	2.15	0.46
1:A:160:ASP:O	1:A:164:ARG:HG2	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLN:HG2	1:A:212:GLU:OE1	2.16	0.45
1:A:53:VAL:HG23	1:A:54:SER:H	1.80	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: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
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:ND2	1:A:537:ASN:H	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:683:GLU:CD	1:A:686[B]:ARG:HH12	2.21	0.43
1:A:495:LEU:HA	1:A:495:LEU:HD23	1.91	0.43
1:A:686[B]:ARG:CB	1:A:686[B]:ARG:HH11	2.27	0.43
1:A:26:LYS:O	1:A:26:LYS:HG3	2.19	0.43
1:A:369:LEU:HA	1:A:369:LEU:HD12	1.84	0.43
1:A:32:LYS:HD2	1:A:51:GLU:OE1	2.19	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:193:VAL:C	3:B:195:PRO:HD3	2.39	0.42
3:B:191:LYS:NZ	4:B:382:HOH:O	2.52	0.42
3:B:95:GLU:OE1	3:B:98[A]:ARG:NH2	2.42	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
1:A:518:ASP:OD1	1:A:518:ASP:C	2.57	0.41
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:HA	3:B:29:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:145:VAL:O	3:B:145:VAL:HG13	2.19	0.41
3:B:16:LEU:O	3:B:20:PHE:HD1	2.03	0.41
1:A:489:LEU:HA	1:A:489:LEU:HD23	1.80	0.41
1:A:35:ILE:HD13	1:A:79:GLN:HG2	2.02	0.41
1:A:134:ILE:O	1:A:154:HIS:HE1	2.02	0.41
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:683:GLU:CD	1:A:686[B]:ARG:NH1	2.73	0.41
1:A:360:GLU:OE1	1:A:370:LYS:HD2	2.21	0.41
1:A:40:ASP:HA	1:A:41:PRO:HD2	1.92	0.41
1:A:623:LYS:O	1:A:625:ALA:N	2.53	0.41
1:A:18:LYS:O	1:A:19:GLN:C	2.59	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
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
3:B:143:VAL:C	3:B:145:VAL:H	2.23	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 (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	782/776 (101%)	744 (95%)	28 (4%)	10 (1%)	12 4
2	L	4/13 (31%)	4 (100%)	0	0	100 100
3	B	300/299 (100%)	283 (94%)	14 (5%)	3 (1%)	15 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1086/1088 (100%)	1031 (95%)	42 (4%)	13 (1%)	13 4

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	205	ALA
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%)	39 30
2	L	6/11 (54%)	6 (100%)	0	100 100
3	B	263/261 (101%)	254 (97%)	9 (3%)	37 28
All	All	957/951 (101%)	926 (97%)	31 (3%)	41 30

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

Mol	Chain	Res	Type
1	A	2	ASN
1	A	54	SER
1	A	66	ASP

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Mol	Chain	Res	Type
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
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	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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	105	ASN
1	A	137	GLN
1	A	154	HIS
1	A	194	GLN
1	A	234	ASN
1	A	271	GLN
1	A	283	GLN
1	A	305	ASN
1	A	385	ASN

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Mol	Chain	Res	Type
1	A	407	GLN
1	A	443	GLN
1	A	484	HIS
1	A	500	ASN
1	A	532	GLN
1	A	537	ASN
1	A	555	ASN
1	A	613	ASN
1	A	616	ASN
1	A	694	ASN
3	B	14	ASN
3	B	25	GLN
3	B	33	GLN
3	B	40	GLN
3	B	75	ASN
3	B	155	GLN
3	B	222	ASN
3	B	278	GLN
3	B	283	GLN
3	B	287	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

There are no carbohydrates 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, 95^{th} 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%)	0.52	68 (8%) 9 11	13, 25, 64, 102	0
2	L	6/13 (46%)	1.52	2 (33%) 0 0	40, 46, 53, 66	0
3	B	299/299 (100%)	0.59	33 (11%) 5 6	18, 31, 63, 76	0
All	All	1069/1088 (98%)	0.55	103 (9%) 8 9	13, 27, 64, 102	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	25	PHE	17.8
1	A	29	VAL	16.7
1	A	621	ALA	14.3
1	A	22	SER	14.1
1	A	20	GLY	11.5
1	A	623	LYS	11.4
1	A	24	LEU	11.1
1	A	27	LEU	11.0
1	A	28	THR	9.9
1	A	23	ASP	9.7
3	B	145	VAL	9.6
1	A	624	GLY	9.6
1	A	620	ARG	9.5
1	A	625	ALA	9.4
1	A	619	SER	9.3
1	A	31	ASP	8.3
3	B	242	ILE	8.2
3	B	148	GLN	8.1
1	A	626	ASN	7.9
1	A	21	ASP	7.4
3	B	110	GLY	7.3
1	A	618	ALA	7.0
3	B	112	ASN	6.8

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Mol	Chain	Res	Type	RSRZ
1	A	19	GLN	6.7
1	A	206	ASN	6.3
3	B	111	THR	6.3
1	A	616	ASN	6.0
1	A	204	GLN	5.8
1	A	203	ASN	5.7
3	B	61	SER	5.5
1	A	363	ALA	5.4
1	A	30	SER	5.4
3	B	244	GLY	5.4
3	B	143	VAL	5.3
1	A	622	LYS	5.3
2	L	771	ARG	5.3
1	A	65	VAL	5.1
1	A	617	ILE	5.0
3	B	243	ASP	5.0
1	A	563	PHE	5.0
1	A	365	GLU	5.0
1	A	627	PHE	4.8
1	A	615	PRO	4.8
1	A	32	LYS	4.4
3	B	144	PRO	4.3
1	A	68	GLN	4.2
1	A	364	GLY	4.1
3	B	239	GLN	4.0
3	B	62	GLY	4.0
1	A	71	GLN	3.9
3	B	240	LYS	3.9
1	A	66	ASP	3.8
3	B	146	GLY	3.7
1	A	362	GLY	3.7
3	B	7	GLU	3.7
1	A	404	LEU	3.6
3	B	224	LEU	3.6
3	B	147	ASP	3.6
1	A	445	ARG	3.5
1	A	520	ARG	3.5
1	A	35	ILE	3.3
1	A	208	SER	3.2
3	B	241	ASP	3.2
1	A	26	LYS	3.1
3	B	149	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
3	B	245	LYS	3.1
3	B	59	ARG	3.1
3	B	60	GLY	3.0
1	A	57	SER	3.0
1	A	62	PHE	2.9
1	A	614	ASP	2.8
3	B	150	PRO	2.8
1	A	403	ASP	2.8
3	B	6	MET	2.8
1	A	462	LYS	2.7
3	B	142	LYS	2.7
3	B	238	SER	2.7
1	A	18	LYS	2.6
1	A	59	SER	2.6
3	B	294	PRO	2.6
1	A	170	ARG	2.6
1	A	316	LYS	2.6
3	B	87	LYS	2.5
1	A	717	GLU	2.5
1	A	393	LEU	2.5
1	A	54	SER	2.5
1	A	53	VAL	2.5
1	A	205	ALA	2.4
1	A	602[A]	ASP	2.4
3	B	204	ILE	2.4
1	A	202	ARG	2.4
1	A	408	HIS	2.3
1	A	61	THR	2.3
1	A	76	ASP	2.3
3	B	298	ASN	2.3
3	B	207	LEU	2.2
1	A	52	ILE	2.2
2	L	770	PRO	2.2
3	B	154	PHE	2.1
1	A	58	ASP	2.1
1	A	2	ASN	2.1
1	A	34	TYR	2.0
1	A	549	SER	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.