



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:26 am BST

PDB ID : 3PN7
Title : Visualizing new hinges and a potential major source of compliance in the lever arm of myosin
Authors : Brown, J.H.; Senthil-Kumar, V.S.; O'Neill-Hennessey, E.; Reshetnikova, L.; Robinson, H.; Nguyen-McCarty, M.; Szent-Gyorgyi, A.G.; Cohen, C.
Deposited on : 2010-11-18
Resolution : 2.25 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

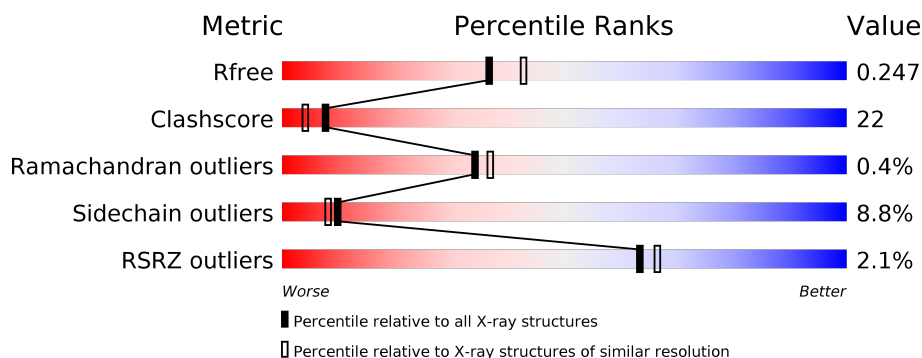
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 $\leq 5\%$. 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	69	<div> <div>74%</div> <div>19%</div> <div>• •</div> </div>
1	D	69	<div> <div>67%</div> <div>28%</div> <div>6%</div> </div>
2	B	161	<div> <div>2%</div> <div>59%</div> <div>26%</div> <div>•</div> <div>12%</div> </div>
2	E	161	<div> <div>6%</div> <div>53%</div> <div>25%</div> <div>11%</div> <div>•</div> <div>10%</div> </div>
3	C	156	<div> <div>71%</div> <div>22%</div> <div>• • •</div> </div>
3	F	156	<div> <div>2%</div> <div>75%</div> <div>20%</div> <div>• •</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6407 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 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	68	Total	C	N	O	S	0	0	0
			598	392	113	91	2			
1	D	69	Total	C	N	O	S	0	0	0
			606	396	115	93	2			

- Molecule 2 is a protein called Myosin regulatory light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	141	Total	C	N	O	S	0	0	0
			1135	718	183	223	11			
2	E	145	Total	C	N	O	S	0	0	0
			1166	739	188	228	11			

- Molecule 3 is a protein called Myosin essential light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	152	Total	C	N	O	S	0	0	0
			1210	764	192	247	7			
3	F	151	Total	C	N	O	S	0	0	0
			1198	755	191	245	7			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Ca 1 1	0	0
5	F	1	Total Ca 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	44	Total O 44 44	0	0
6	B	115	Total O 115 115	0	0
6	C	121	Total O 121 121	0	0
6	D	46	Total O 46 46	0	0
6	E	60	Total O 60 60	0	0
6	F	104	Total O 104 104	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 heavy chain

Chain A: 



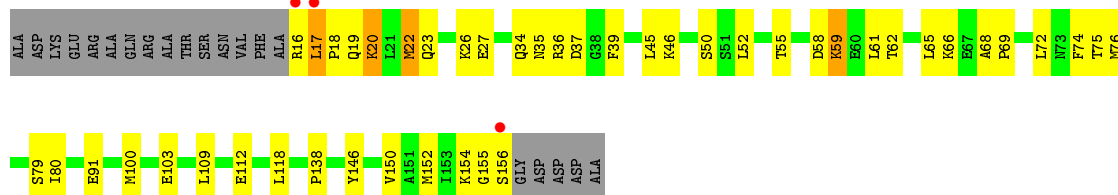
- Molecule 1: Myosin heavy chain

Chain D: 



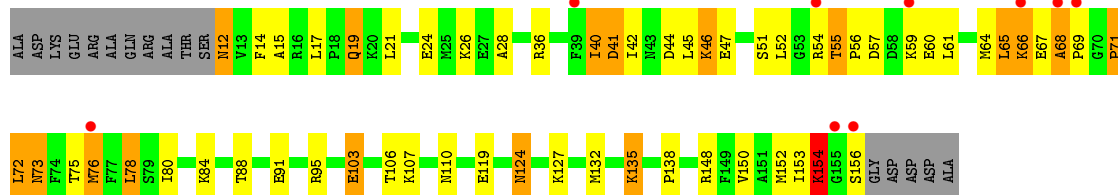
- Molecule 2: Myosin regulatory light chain

Chain B: 



- Molecule 2: Myosin regulatory light chain

Chain E: 

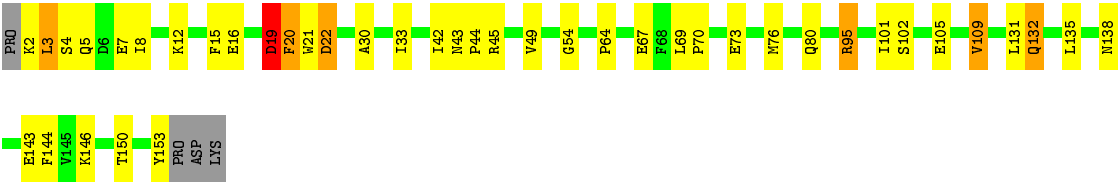


- Molecule 3: Myosin essential light chain

Chain C:

71%

22%



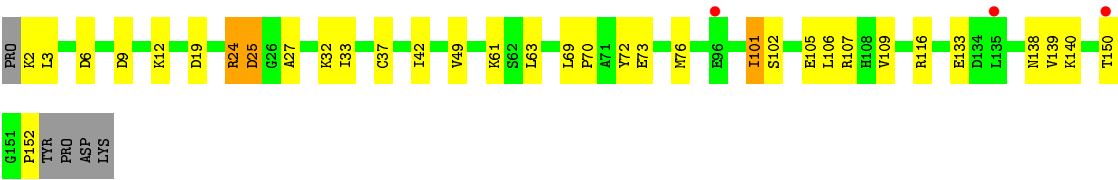
• Molecule 3: Myosin essential light chain

Chain F:

2%

75%

20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.74Å 68.78Å 79.31Å 77.41° 85.94° 73.61°	Depositor
Resolution (Å)	48.67 – 2.25 48.67 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.2 (48.67-2.25) 95.2 (48.67-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 2009_12_14_1757)	Depositor
R, R_{free}	0.191 , 0.241 0.212 , 0.247	Depositor DCC
R_{free} test set	2000 reflections (4.21%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6407	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MG

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	0.47	0/611	0.56	1/818 (0.1%)
1	D	0.37	0/619	0.49	0/829
2	B	0.42	0/1153	0.60	0/1540
2	E	0.43	0/1185	0.57	1/1584 (0.1%)
3	C	0.48	0/1233	0.59	1/1658 (0.1%)
3	F	0.52	2/1220 (0.2%)	0.60	0/1640
All	All	0.46	2/6021 (0.0%)	0.58	3/8069 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	25	ASP	C-N	-6.55	1.21	1.33
3	F	116	ARG	C-N	-5.86	1.20	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	19	ASP	O-C-N	-5.92	113.23	122.70
2	E	124	ASN	CB-CA-C	-5.51	99.38	110.40
1	A	821	LEU	CA-CB-CG	5.45	127.83	115.30

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	598	0	643	18	0
1	D	606	0	649	24	0
2	B	1135	0	1118	57	0
2	E	1166	0	1147	97	0
3	C	1210	0	1133	40	0
3	F	1198	0	1123	32	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
6	A	44	0	0	4	0
6	B	115	0	0	18	0
6	C	121	0	0	11	0
6	D	46	0	0	13	0
6	E	60	0	0	7	0
6	F	104	0	0	8	0
All	All	6407	0	5813	257	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 22.

All (257) 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)
2:B:16:ARG:CB	2:B:17:LEU:HA	1.48	1.41
2:B:16:ARG:HB3	2:B:17:LEU:CA	1.49	1.38
3:F:24:ARG:HG2	3:F:24:ARG:HH11	1.05	1.19
2:E:84:LYS:HB2	6:E:700:HOH:O	1.41	1.18
2:E:69:PRO:CD	2:E:76:MET:HG2	1.76	1.16
2:E:88:THR:HG23	2:E:156:SER:HB2	1.25	1.14
2:E:69:PRO:CG	2:E:76:MET:HG2	1.79	1.12
2:E:19:GLN:HE21	2:E:19:GLN:HA	1.14	1.12
2:E:69:PRO:HD2	2:E:76:MET:HG2	1.29	1.11
2:E:88:THR:CG2	2:E:156:SER:HB2	1.81	1.09
2:B:16:ARG:HD3	2:B:18:PRO:HD3	1.16	1.09
3:C:3:LEU:HB2	6:C:780:HOH:O	1.50	1.09
2:B:16:ARG:HD3	2:B:18:PRO:CD	1.83	1.08
1:A:777:ARG:HD2	6:A:838:HOH:O	1.51	1.08
2:E:153:ILE:O	2:E:154:LYS:HB2	1.53	1.07
3:F:42:ILE:HG22	6:F:839:HOH:O	1.54	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:71:PRO:HG2	2:E:76:MET:SD	1.96	1.04
3:C:12:LYS:HE2	6:C:785:HOH:O	1.58	1.00
1:D:819:LEU:HB2	6:D:842:HOH:O	1.60	1.00
2:E:71:PRO:O	2:E:76:MET:SD	2.20	1.00
2:B:16:ARG:CD	2:B:18:PRO:HD3	1.92	0.99
2:E:91:GLU:HB3	2:E:95:ARG:HH21	1.29	0.97
2:E:69:PRO:CG	2:E:76:MET:CG	2.42	0.97
3:F:24:ARG:HG2	3:F:24:ARG:NH1	1.73	0.97
2:B:16:ARG:HD2	6:B:771:HOH:O	1.62	0.97
2:B:68:ALA:HB2	2:B:80:ILE:HD11	1.49	0.94
2:E:71:PRO:HG2	2:E:76:MET:CE	1.97	0.94
1:D:819:LEU:HD12	6:D:842:HOH:O	1.67	0.93
2:B:154:LYS:HD3	6:B:740:HOH:O	1.74	0.88
2:E:69:PRO:HG2	2:E:76:MET:HG2	1.57	0.86
2:E:42:ILE:HD12	2:E:42:ILE:H	1.40	0.85
2:B:16:ARG:HB2	6:B:771:HOH:O	1.79	0.83
2:E:69:PRO:HG2	2:E:76:MET:CG	2.09	0.82
1:D:816:ARG:HA	6:D:842:HOH:O	1.78	0.81
2:B:16:ARG:CD	6:B:771:HOH:O	2.20	0.80
3:C:2:LYS:HD3	3:C:76:MET:HE1	1.63	0.79
2:E:42:ILE:HG13	2:E:65:LEU:HD23	1.64	0.79
2:B:16:ARG:CB	6:B:771:HOH:O	2.28	0.79
6:D:843:HOH:O	2:E:132:MET:CE	2.30	0.78
2:B:62:THR:O	2:B:66:LYS:HG3	1.85	0.77
2:B:16:ARG:HD3	2:B:18:PRO:CG	2.16	0.76
3:C:5:GLN:NE2	3:C:5:GLN:HA	2.02	0.75
3:C:33:ILE:HD12	3:C:54:GLY:HA2	1.68	0.75
2:E:110:ASN:HB3	6:E:219:HOH:O	1.87	0.74
2:E:153:ILE:O	2:E:154:LYS:CE	2.36	0.74
2:E:57:ASP:OD2	2:E:59:LYS:HB2	1.86	0.73
1:D:822:ARG:HB3	6:D:845:HOH:O	1.89	0.73
3:C:5:GLN:HE21	3:C:5:GLN:HA	1.53	0.72
3:F:24:ARG:HH11	3:F:24:ARG:CG	1.89	0.72
2:E:84:LYS:HD3	6:E:700:HOH:O	1.90	0.72
6:D:843:HOH:O	2:E:132:MET:HE1	1.88	0.72
3:C:146:LYS:O	3:C:150:THR:HG23	1.90	0.71
1:D:805:ARG:HD2	6:D:840:HOH:O	1.91	0.71
1:D:836:LEU:HD11	2:E:52:LEU:HD21	1.72	0.71
2:E:153:ILE:O	2:E:154:LYS:HE3	1.91	0.71
2:E:153:ILE:C	2:E:154:LYS:HE2	2.11	0.71
2:E:69:PRO:CD	2:E:76:MET:CG	2.63	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:69:PRO:HD2	2:E:76:MET:CG	2.16	0.70
2:E:67:GLU:O	2:E:68:ALA:HB3	1.92	0.70
2:B:17:LEU:N	2:B:17:LEU:HD23	2.05	0.69
2:B:16:ARG:HB3	2:B:17:LEU:C	2.13	0.68
2:E:19:GLN:NE2	2:E:19:GLN:HA	1.97	0.67
2:B:16:ARG:HB3	2:B:17:LEU:HA	0.71	0.67
1:D:778:LEU:O	1:D:782:ILE:HG12	1.95	0.67
2:B:91:GLU:HG3	2:B:150:VAL:HG12	1.77	0.65
2:E:66:LYS:HB2	2:E:66:LYS:NZ	2.11	0.65
2:B:16:ARG:CB	2:B:17:LEU:CA	2.29	0.65
3:F:102:SER:HB2	3:F:105:GLU:H	1.60	0.65
1:D:819:LEU:CD1	6:D:842:HOH:O	2.36	0.65
2:B:35:ASN:HB3	2:B:37:ASP:HB2	1.78	0.65
3:F:12:LYS:NZ	6:F:176:HOH:O	2.30	0.64
1:D:819:LEU:HA	1:D:822:ARG:HD2	1.80	0.64
2:E:42:ILE:N	2:E:42:ILE:HD12	2.10	0.64
1:D:818:TRP:CD2	2:E:153:ILE:HG22	2.33	0.64
3:C:20:PHE:C	3:C:20:PHE:CD1	2.71	0.63
1:D:819:LEU:CG	6:D:842:HOH:O	2.45	0.63
2:B:91:GLU:HG3	2:B:150:VAL:CG1	2.29	0.63
1:A:836:LEU:O	1:A:837:LEU:HB2	1.98	0.62
2:E:69:PRO:HG2	2:E:76:MET:CE	2.28	0.62
2:E:71:PRO:HG2	2:E:76:MET:HE2	1.80	0.62
3:C:69:LEU:HB3	3:C:70:PRO:HD3	1.81	0.62
2:B:35:ASN:CB	2:B:37:ASP:HB2	2.30	0.61
2:B:58:ASP:O	2:B:62:THR:HG23	1.99	0.61
2:E:88:THR:HG21	2:E:156:SER:HB2	1.79	0.61
2:E:153:ILE:O	2:E:154:LYS:HE2	1.98	0.61
2:E:91:GLU:HB3	2:E:95:ARG:NH2	2.09	0.61
3:F:2:LYS:HB3	6:F:587:HOH:O	2.00	0.61
1:D:801:LEU:HD12	6:D:841:HOH:O	1.99	0.60
2:E:42:ILE:CD1	2:E:42:ILE:H	2.13	0.60
2:E:61:LEU:O	2:E:65:LEU:HB2	2.02	0.60
2:E:69:PRO:HG3	2:E:76:MET:HG3	1.83	0.60
1:D:830:TYR:HE2	1:D:834:LYS:HE2	1.65	0.60
2:E:69:PRO:O	2:E:71:PRO:HD2	2.02	0.59
1:A:780:LYS:HE3	3:C:45:ARG:NH1	2.18	0.59
2:E:41:ASP:H	2:E:44:ASP:HB2	1.69	0.58
2:B:16:ARG:HB2	2:B:17:LEU:HA	1.71	0.58
3:F:2:LYS:HG3	3:F:76:MET:HE1	1.85	0.58
2:E:40:ILE:CD1	2:E:45:LEU:HD13	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:SER:CA	6:B:728:HOH:O	2.50	0.58
3:C:5:GLN:HE21	3:C:5:GLN:CA	2.14	0.57
1:D:822:ARG:HB3	6:D:844:HOH:O	2.04	0.57
3:F:24:ARG:CG	3:F:24:ARG:NH1	2.55	0.57
6:D:843:HOH:O	2:E:132:MET:HE3	1.99	0.57
3:F:73:GLU:HA	3:F:76:MET:HE2	1.87	0.57
2:B:16:ARG:HB3	2:B:18:PRO:HD3	1.86	0.56
2:E:73:ASN:HD22	2:E:76:MET:HB2	1.70	0.56
2:E:91:GLU:HG2	2:E:150:VAL:HG12	1.86	0.56
2:E:69:PRO:CG	2:E:76:MET:HG3	2.32	0.56
2:E:60:GLU:O	2:E:64:MET:HG2	2.06	0.56
2:B:138:PRO:HD3	6:B:779:HOH:O	2.05	0.55
2:B:19:GLN:O	2:B:23:GLN:HG3	2.05	0.55
2:E:66:LYS:HB2	2:E:66:LYS:HZ1	1.71	0.55
2:B:69:PRO:HD2	2:B:76:MET:SD	2.46	0.55
3:C:3:LEU:N	6:C:780:HOH:O	2.29	0.55
3:F:37:CYS:HB3	3:F:42:ILE:HD11	1.88	0.55
2:B:16:ARG:CG	2:B:18:PRO:HD3	2.36	0.55
3:C:30:ALA:O	3:C:33:ILE:HD12	2.06	0.55
2:E:69:PRO:HG2	2:E:76:MET:HE2	1.89	0.55
2:B:146:TYR:O	2:B:150:VAL:HG23	2.07	0.55
3:F:3:LEU:HD13	3:F:73:GLU:HG2	1.88	0.55
2:E:127:LYS:NZ	2:E:127:LYS:HB3	2.21	0.55
3:F:101:ILE:HG12	3:F:102:SER:N	2.21	0.55
2:E:69:PRO:C	2:E:71:PRO:HD2	2.27	0.54
2:E:84:LYS:CD	6:E:700:HOH:O	2.51	0.54
1:A:770:LEU:HD12	1:A:770:LEU:N	2.22	0.54
2:B:156:SER:HA	6:B:728:HOH:O	2.08	0.54
2:E:84:LYS:CB	6:E:700:HOH:O	2.21	0.54
3:F:25:ASP:O	3:F:27:ALA:N	2.40	0.54
1:D:783:SER:HA	1:D:786:GLN:OE1	2.07	0.53
2:B:154:LYS:CD	6:B:740:HOH:O	2.46	0.53
2:B:55:THR:HG23	6:B:613:HOH:O	2.08	0.53
2:E:76:MET:O	2:E:80:ILE:HG23	2.08	0.53
2:B:154:LYS:CE	6:B:740:HOH:O	2.56	0.53
1:A:801:LEU:HG	3:C:21:TRP:NE1	2.24	0.52
1:D:769:ASN:HB3	1:D:772:GLU:HB2	1.91	0.52
2:E:67:GLU:O	2:E:68:ALA:CB	2.54	0.52
3:C:73:GLU:HA	3:C:76:MET:HE2	1.91	0.52
1:A:834:LYS:HD3	6:B:557:HOH:O	2.09	0.52
1:D:805:ARG:NE	6:D:119:HOH:O	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:133:GLU:HA	3:F:138:ASN:O	2.10	0.52
2:B:152:MET:SD	6:B:779:HOH:O	2.59	0.52
3:C:3:LEU:CB	6:C:780:HOH:O	2.27	0.51
1:A:801:LEU:HG	3:C:21:TRP:HE1	1.75	0.51
2:E:69:PRO:HG2	2:E:76:MET:SD	2.50	0.51
3:F:42:ILE:CG2	6:F:839:HOH:O	2.31	0.51
2:E:15:ALA:HB3	6:E:809:HOH:O	2.10	0.51
2:E:66:LYS:C	2:E:68:ALA:H	2.14	0.51
2:E:14:PHE:CE2	2:E:75:THR:HG22	2.46	0.51
1:D:800:LYS:NZ	2:E:103:GLU:OE1	2.34	0.51
1:A:828:LYS:NZ	6:A:379:HOH:O	2.43	0.50
2:E:40:ILE:HD13	2:E:45:LEU:HD13	1.93	0.50
3:F:3:LEU:CD1	3:F:73:GLU:HG2	2.42	0.50
3:C:22:ASP:OD2	3:C:22:ASP:O	2.30	0.50
2:E:106:THR:O	2:E:107:LYS:HB2	2.12	0.49
3:F:32:LYS:HE3	6:F:303:HOH:O	2.11	0.49
2:E:73:ASN:N	2:E:73:ASN:HD22	2.09	0.49
2:E:152:MET:O	2:E:154:LYS:HE2	2.12	0.49
2:E:73:ASN:HD22	2:E:73:ASN:H	1.60	0.49
3:F:69:LEU:HB3	3:F:70:PRO:HD3	1.95	0.49
2:B:46:LYS:HG2	2:B:61:LEU:CD1	2.43	0.48
1:D:834:LYS:N	1:D:835:PRO:CD	2.76	0.48
2:E:119:GLU:O	2:E:124:ASN:HB3	2.13	0.48
2:E:42:ILE:HG22	2:E:46:LYS:HD3	1.96	0.48
2:B:19:GLN:NE2	6:B:766:HOH:O	2.46	0.48
3:C:16:GLU:HG2	6:C:651:HOH:O	2.13	0.48
2:E:66:LYS:NZ	2:E:66:LYS:CB	2.77	0.48
1:D:770:LEU:O	1:D:774:ARG:HG3	2.14	0.48
2:E:73:ASN:ND2	2:E:76:MET:HB2	2.29	0.48
3:F:33:ILE:HD11	3:F:63:LEU:HD11	1.96	0.48
1:A:821:LEU:HG	1:A:827:TRP:CG	2.49	0.47
3:C:19:ASP:OD1	3:C:19:ASP:O	2.30	0.47
1:A:818:TRP:HA	1:A:821:LEU:HD22	1.95	0.47
2:B:16:ARG:CB	2:B:18:PRO:HD3	2.43	0.47
2:B:37:ASP:HB3	2:B:39:PHE:H	1.79	0.47
3:C:131:LEU:HD13	3:C:144:PHE:HB2	1.96	0.47
2:E:17:LEU:HD23	2:E:21:LEU:HD22	1.96	0.47
1:D:769:ASN:HB3	1:D:772:GLU:CB	2.44	0.47
3:F:150:THR:HG22	3:F:150:THR:O	2.14	0.47
3:C:3:LEU:HD13	3:C:73:GLU:HG2	1.96	0.47
2:B:45:LEU:HD22	2:B:65:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:15:ALA:CB	6:E:809:HOH:O	2.63	0.47
3:F:19:ASP:OD1	3:F:25:ASP:O	2.33	0.47
2:B:22:MET:HE1	6:B:766:HOH:O	2.14	0.47
2:B:155:GLY:O	2:B:156:SER:HB3	2.15	0.47
2:B:16:ARG:NH1	6:B:772:HOH:O	2.30	0.46
1:D:830:TYR:OH	2:E:24:GLU:OE1	2.23	0.46
2:E:64:MET:O	2:E:67:GLU:HG3	2.15	0.46
3:C:12:LYS:CE	6:C:785:HOH:O	2.37	0.46
2:E:40:ILE:HD12	2:E:41:ASP:O	2.16	0.46
2:B:35:ASN:C	2:B:37:ASP:H	2.17	0.46
2:E:42:ILE:O	2:E:46:LYS:HG2	2.15	0.46
1:A:823:ASN:HB2	6:A:628:HOH:O	2.14	0.46
1:D:796:LYS:HD3	3:F:152:PRO:HB3	1.97	0.46
3:C:95:ARG:HB3	3:C:95:ARG:NH1	2.31	0.46
2:E:78:LEU:HD12	2:E:78:LEU:HA	1.79	0.46
3:F:106:LEU:O	3:F:109:VAL:HG22	2.15	0.46
2:B:35:ASN:C	2:B:37:ASP:N	2.68	0.45
3:C:49:VAL:CG2	6:C:501:HOH:O	2.64	0.45
1:A:804:GLN:HA	2:B:100:MET:HG2	1.98	0.45
2:B:50:SER:HA	2:B:55:THR:HG22	1.99	0.45
2:B:16:ARG:HB3	2:B:18:PRO:CD	2.46	0.45
3:C:42:ILE:HG13	3:C:44:PRO:HD3	1.99	0.45
2:E:138:PRO:HB3	2:E:148:ARG:NH2	2.32	0.45
1:A:770:LEU:HD13	6:A:364:HOH:O	2.17	0.44
1:A:821:LEU:HG	1:A:827:TRP:CD2	2.52	0.44
2:B:155:GLY:O	2:B:156:SER:CB	2.65	0.44
3:C:101:ILE:HG12	3:C:105:GLU:HB2	1.97	0.44
3:C:45:ARG:HD3	6:C:669:HOH:O	2.17	0.44
2:E:42:ILE:HG13	2:E:65:LEU:CD2	2.43	0.44
2:E:65:LEU:HD12	2:E:72:LEU:HD12	1.98	0.44
3:F:37:CYS:SG	3:F:72:TYR:HD1	2.41	0.44
2:E:40:ILE:HG13	2:E:40:ILE:O	2.17	0.44
1:A:821:LEU:C	1:A:821:LEU:HD23	2.39	0.43
3:C:143:GLU:OE1	6:C:752:HOH:O	2.21	0.43
3:C:105:GLU:O	3:C:109:VAL:HG13	2.17	0.43
2:E:71:PRO:CG	2:E:76:MET:HE2	2.47	0.43
3:C:16:GLU:HG3	6:C:785:HOH:O	2.17	0.43
2:E:21:LEU:HD23	2:E:21:LEU:C	2.38	0.43
2:E:55:THR:HA	2:E:56:PRO:HD3	1.89	0.43
3:F:101:ILE:CG2	3:F:139:VAL:HG23	2.49	0.43
2:B:35:ASN:O	2:B:36:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:91:GLU:HG3	2:E:154:LYS:O	2.19	0.43
3:C:4:SER:OG	3:C:7:GLU:HG3	2.18	0.43
3:C:102:SER:HA	3:C:138:ASN:HD22	1.84	0.43
2:B:68:ALA:HB1	2:B:76:MET:CG	2.49	0.43
3:F:61:LYS:HE2	3:F:63:LEU:HD21	2.00	0.43
1:D:837:LEU:HD11	2:E:28:ALA:HB2	2.01	0.42
2:E:21:LEU:O	2:E:21:LEU:HD23	2.19	0.42
2:B:22:MET:CE	6:B:766:HOH:O	2.67	0.42
3:F:101:ILE:HG23	3:F:139:VAL:HG23	2.01	0.42
1:A:801:LEU:HG	3:C:21:TRP:CD1	2.54	0.42
2:E:19:GLN:CA	2:E:19:GLN:HE21	1.98	0.42
3:F:107:ARG:NH2	6:F:689:HOH:O	2.52	0.42
2:B:20:LYS:HB3	2:B:20:LYS:NZ	2.35	0.42
3:C:43:ASN:H	3:C:80:GLN:NE2	2.18	0.42
2:E:71:PRO:CG	2:E:76:MET:CE	2.82	0.42
3:F:106:LEU:O	3:F:109:VAL:CG2	2.68	0.42
3:F:140:LYS:N	6:F:831:HOH:O	2.40	0.42
1:A:834:LYS:HB3	1:A:835:PRO:HD3	2.02	0.41
1:A:793:LEU:HD12	1:A:793:LEU:HA	1.92	0.41
3:C:15:PHE:O	3:C:19:ASP:N	2.48	0.41
3:C:64:PRO:HD2	3:C:67:GLU:HB2	2.02	0.41
3:C:5:GLN:HE22	3:C:8:ILE:HD12	1.85	0.41
2:E:59:LYS:HE2	2:E:59:LYS:HB3	1.98	0.41
2:B:35:ASN:HB2	2:B:37:ASP:HB2	2.03	0.41
2:E:12:ASN:OD1	2:E:12:ASN:C	2.59	0.41
2:E:135:LYS:HB2	2:E:135:LYS:NZ	2.36	0.41
2:B:59:LYS:HD2	2:B:59:LYS:HA	1.71	0.41
2:B:34:GLN:HB3	6:B:706:HOH:O	2.20	0.41
3:C:132:GLN:HG2	6:C:164:HOH:O	2.21	0.41
2:E:36:ARG:HD3	2:E:36:ARG:HA	1.96	0.41
2:E:54:ARG:H	2:E:54:ARG:HG3	1.65	0.40
2:E:68:ALA:HA	2:E:69:PRO:HA	1.79	0.40
2:E:73:ASN:ND2	2:E:76:MET:H	2.20	0.40
2:B:26:LYS:HA	2:B:74:PHE:CE1	2.56	0.40
3:F:9:ASP:HB3	6:F:463:HOH:O	2.21	0.40
3:C:21:TRP:CE3	3:C:21:TRP:HA	2.56	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	66/69 (96%)	66 (100%)	0	0	100	100
1	D	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
2	B	139/161 (86%)	134 (96%)	5 (4%)	0	100	100
2	E	143/161 (89%)	130 (91%)	10 (7%)	3 (2%)	7	3
3	C	150/156 (96%)	146 (97%)	4 (3%)	0	100	100
3	F	149/156 (96%)	142 (95%)	7 (5%)	0	100	100
All	All	714/772 (92%)	684 (96%)	27 (4%)	3 (0%)	34	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	154	LYS
2	E	68	ALA
2	E	71	PRO

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	63/64 (98%)	57 (90%)	6 (10%)	8	6
1	D	64/64 (100%)	58 (91%)	6 (9%)	8	6
2	B	126/140 (90%)	113 (90%)	13 (10%)	7	5
2	E	129/140 (92%)	111 (86%)	18 (14%)	3	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	129/133 (97%)	120 (93%)	9 (7%)	15	13
3	F	128/133 (96%)	124 (97%)	4 (3%)	40	49
All	All	639/674 (95%)	583 (91%)	56 (9%)	10	8

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	770	LEU
1	A	777	ARG
1	A	779	SER
1	A	788	HIS
1	A	793	LEU
1	A	821	LEU
2	B	17	LEU
2	B	20	LYS
2	B	22	MET
2	B	27	GLU
2	B	52	LEU
2	B	59	LYS
2	B	72	LEU
2	B	75	THR
2	B	79	SER
2	B	103	GLU
2	B	109	LEU
2	B	112	GLU
2	B	118	LEU
3	C	3	LEU
3	C	19	ASP
3	C	20	PHE
3	C	22	ASP
3	C	95	ARG
3	C	109	VAL
3	C	132	GLN
3	C	135	LEU
3	C	153	TYR
1	D	770	LEU
1	D	772	GLU
1	D	780	LYS
1	D	788	HIS
1	D	805	ARG
1	D	822	ARG

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Mol	Chain	Res	Type
2	E	12	ASN
2	E	19	GLN
2	E	26	LYS
2	E	40	ILE
2	E	41	ASP
2	E	46	LYS
2	E	47	GLU
2	E	51	SER
2	E	55	THR
2	E	65	LEU
2	E	66	LYS
2	E	72	LEU
2	E	73	ASN
2	E	76	MET
2	E	78	LEU
2	E	103	GLU
2	E	135	LYS
2	E	154	LYS
3	F	6	ASP
3	F	24	ARG
3	F	49	VAL
3	F	101	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	19	GLN
2	B	34	GLN
2	B	35	ASN
2	B	96	ASN
3	C	5	GLN
3	C	132	GLN
3	C	138	ASN
2	E	19	GLN
2	E	23	GLN
2	E	73	ASN
2	E	96	ASN
2	E	120	ASN
3	F	80	GLN
3	F	132	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	68/69 (98%)	-0.01	0 100 100	25, 34, 54, 66	0
1	D	69/69 (100%)	-0.18	0 100 100	20, 39, 75, 82	0
2	B	141/161 (87%)	0.01	3 (2%) 63 66	20, 37, 58, 74	0
2	E	145/161 (90%)	0.28	9 (6%) 20 22	20, 49, 81, 92	0
3	C	152/156 (97%)	-0.06	0 100 100	25, 37, 57, 68	0
3	F	151/156 (96%)	0.05	3 (1%) 65 68	20, 45, 84, 98	0
All	All	726/772 (94%)	0.04	15 (2%) 63 66	20, 40, 74, 98	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	69	PRO	6.3
2	B	16	ARG	6.3
3	F	135	LEU	6.2
2	E	68	ALA	4.2
2	E	156	SER	3.7
2	E	54	ARG	3.5
2	B	156	SER	3.2
2	E	59	LYS	3.0
2	B	17	LEU	2.9
3	F	96	GLU	2.9
2	E	39	PHE	2.6
2	E	76	MET	2.5
2	E	66	LYS	2.4
2	E	155	GLY	2.2
3	F	150	THR	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	B	162	1/1	0.74	0.31	44,44,44,44	0
4	MG	E	162	1/1	0.84	0.10	67,67,67,67	0
5	CA	C	157	1/1	0.96	0.06	46,46,46,46	0
5	CA	F	157	1/1	0.99	0.11	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.