



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:20 PM UTC

PDB ID : 3PN7 / pdb_00003pn7
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 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:

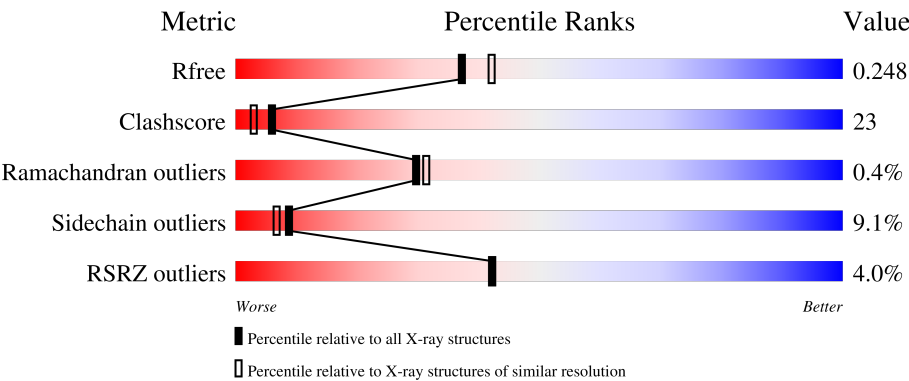
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 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	69	3% 72% 22% ..
1	D	69	% 67% 28% 6%
2	B	161	4% 58% 27% • 12%
2	E	161	8% 53% 25% 12% • 10%
3	C	156	% 69% 22% 5% ..

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Mol	Chain	Length	Quality of chain
3	F	156	3% 72% 22% ...

2 Entry composition [i](#)

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 (CCD ID: MG) (formula: Mg).

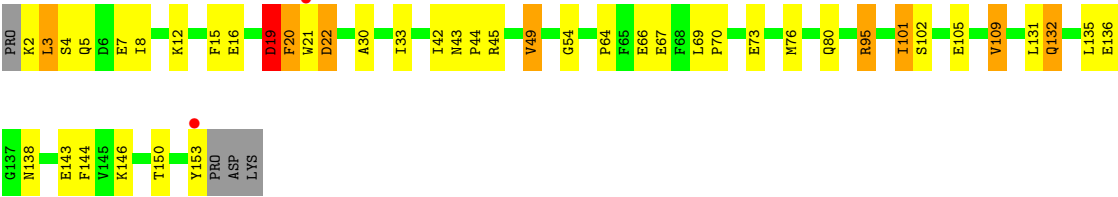
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 6 is water.

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



● Molecule 3: Myosin essential light chain



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 0.213 , 0.248	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 , 33.0	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	0.62	1/611 (0.2%)	0.82	0/818
1	D	0.47	0/619	0.79	0/829
2	B	0.51	0/1153	0.87	3/1540 (0.2%)
2	E	0.54	2/1185 (0.2%)	0.83	2/1584 (0.1%)
3	C	0.58	1/1233 (0.1%)	0.86	1/1658 (0.1%)
3	F	0.69	4/1220 (0.3%)	0.86	4/1640 (0.2%)
All	All	0.58	8/6021 (0.1%)	0.84	10/8069 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	116	ARG	C-N	-9.37	1.20	1.33
3	F	18	PHE	C-N	-8.40	1.22	1.33
3	F	25	ASP	C-N	-8.38	1.21	1.33
2	E	75	THR	C-N	-8.13	1.22	1.33
3	F	19	ASP	C-N	-7.07	1.25	1.33
3	C	19	ASP	C-N	-6.61	1.24	1.33
1	A	831	ALA	C-N	-6.56	1.24	1.33
2	E	89	ASP	C-N	-6.31	1.24	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	124	ASN	CB-CA-C	-7.68	99.38	110.06
3	F	25	ASP	O-C-N	-7.29	115.84	123.56
3	C	19	ASP	O-C-N	-6.69	113.23	122.46
2	B	36	ARG	N-CA-C	-6.34	105.96	113.38
2	E	124	ASN	N-CA-C	6.28	119.71	110.30
2	B	38	GLY	N-CA-C	-5.75	107.17	115.27
3	F	104	ALA	N-CA-C	-5.44	107.65	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	24	ARG	O-C-N	-5.32	115.52	122.59
2	B	19	GLN	N-CA-C	5.30	117.74	111.33
3	F	103	GLY	N-CA-C	-5.23	108.49	115.40

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	19	0
1	D	606	0	649	24	0
2	B	1135	0	1118	61	0
2	E	1166	0	1147	100	0
3	C	1210	0	1134	42	0
3	F	1198	0	1125	34	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	19	0
6	C	121	0	0	11	0
6	D	46	0	0	12	0
6	E	60	0	0	7	0
6	F	104	0	0	9	0
All	All	6407	0	5816	268	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 23.

All (268) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:ARG:HB3	2:B:17:LEU:CA	1.49	1.38
3:F:24:ARG:HH11	3:F:24:ARG:HG2	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
6:D:843:HOH:O	2:E:132:MET:HE1	1.53	1.08
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
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
2:B:22:MET:HE1	6:F:765:HOH:O	1.82	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
3:C:2:LYS:HD3	3:C:76:MET:HE1	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:69:PRO:HG2	2:E:76:MET:HE2	1.67	0.76
2:E:153:ILE:C	2:E:154:LYS:HE2	2.11	0.76
3:C:5:GLN:HA	3:C:5:GLN:NE2	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
2:B:16:ARG:HB3	2:B:17:LEU:C	2.13	0.73
1:D:822:ARG:HB3	6:D:845:HOH:O	1.89	0.73
3:C:5:GLN:HA	3:C:5:GLN:HE21	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
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:69:PRO:CD	2:E:76:MET:CG	2.63	0.71
2:E:69:PRO:HD2	2:E:76:MET:CG	2.16	0.70
2:B:17:LEU:N	2:B:17:LEU:HD23	2.05	0.69
1:D:819:LEU:HD22	2:E:132:MET:HE2	1.74	0.69
3:C:20:PHE:C	3:C:20:PHE:CD1	2.71	0.68
2:E:19:GLN:HA	2:E:19:GLN:NE2	1.97	0.67
2:E:67:GLU:O	2:E:68:ALA:HB3	1.92	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
3:F:73:GLU:HA	3:F:76:MET:HE2	1.78	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:HD12	2:E:42:ILE:N	2.10	0.64
1:D:818:TRP:CD2	2:E:153:ILE:HG22	2.33	0.64
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
3:C:69:LEU:HB3	3:C:70:PRO:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:2:LYS:HG3	3:F:76:MET:HE1	1.83	0.60
1:D:801:LEU:HD12	6:D:841:HOH:O	1.99	0.60
2:E:42:ILE:H	2:E:42:ILE:CD1	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
2:E:69:PRO:C	2:E:71:PRO:HD2	2.27	0.59
2:E:71:PRO:HG2	2:E:76:MET:HE1	1.85	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
2:E:40:ILE:CD1	2:E:45:LEU:HD13	2.33	0.58
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:NH1	3:F:24:ARG:CG	2.55	0.57
6:D:843:HOH:O	2:E:132:MET:CE	2.30	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:69:PRO:CG	2:E:76:MET:HG3	2.32	0.56
2:E:91:GLU:HG2	2:E:150:VAL:HG12	1.86	0.56
2:E:60:GLU:O	2:E:64:MET:HG2	2.06	0.56
2:E:66:LYS:C	2:E:68:ALA:H	2.14	0.56
2:B:19:GLN:O	2:B:23:GLN:HG3	2.05	0.55
2:B:138:PRO:HD3	6:B:779:HOH:O	2.05	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: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
2:E:84:LYS:CD	6:E:700:HOH:O	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:LEU:HD12	1:A:770:LEU:N	2.22	0.54
3:F:101:ILE:HG12	3:F:102:SER:N	2.21	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:55:THR:HG23	6:B:613:HOH:O	2.08	0.53
2:B:154:LYS:CD	6:B:740:HOH:O	2.46	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
2:B:22:MET:HE2	6:B:766:HOH:O	2.09	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
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:B:35:ASN:C	2:B:37:ASP:H	2.17	0.51
2:E:15:ALA:HB3	6:E:809:HOH:O	2.10	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
2:E:69:PRO:CG	2:E:76:MET:HE2	2.37	0.51
1:A:828:LYS:NZ	6:A:379:HOH:O	2.43	0.50
2:E:100:MET:HE2	2:E:100:MET:HA	1.93	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:O	3:C:22:ASP:OD2	2.30	0.50
2:B:35:ASN:C	2:B:37:ASP:N	2.68	0.49
3:F:32:LYS:HE3	6:F:303:HOH:O	2.11	0.49
2:E:73:ASN:HD22	2:E:73:ASN:N	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:42:ILE:HG22	2:E:46:LYS:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:119:GLU:O	2:E:124:ASN:HB3	2.13	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
2:E:21:LEU:C	2:E:21:LEU:HD23	2.38	0.48
2:E:106:THR:O	2:E:107:LYS:HB2	2.12	0.48
1:A:821:LEU:C	1:A:821:LEU:HD23	2.39	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: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
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
3:F:150:THR:O	3:F:150:THR:HG22	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
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: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:NH1	3:C:95:ARG:HB3	2.31	0.46
2:E:12:ASN:OD1	2:E:12:ASN:C	2.59	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:LYS:HA	2:B:62:THR:HG1	1.82	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:45:ARG:HD3	6:C:669:HOH:O	2.17	0.44
3:C:101:ILE:HG12	3:C:105:GLU:HB2	1.97	0.44
2:E:42:ILE:HG13	2:E:65:LEU:CD2	2.43	0.44
2:E:88:THR:HG21	2:E:156:SER:C	2.43	0.44
3:F:134:ASP:C	3:F:134:ASP:OD1	2.60	0.44
2:E:65:LEU:HD12	2:E:72:LEU:HD12	1.98	0.44
2:E:66:LYS:HB2	2:E:66:LYS:HZ1	1.82	0.44
3:F:37:CYS:SG	3:F:72:TYR:HD1	2.41	0.44
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
3:F:134:ASP:O	3:F:135:LEU:C	2.60	0.43
3:C:16:GLU:HG3	6:C:785:HOH:O	2.17	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
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:66:GLU:H	3:C:66:GLU:CD	2.26	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
2:B:156:SER:C	6:B:728:HOH:O	2.62	0.42
1:D:837:LEU:HD11	2:E:28:ALA:HB2	2.01	0.42
2:E:21:LEU:HD23	2:E:21:LEU:O	2.19	0.42
2:E:40:ILE:O	2:E:40:ILE:HG13	2.17	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:HE21	2:E:19:GLN:CA	1.98	0.42
3:F:107:ARG:NH2	6:F:689:HOH:O	2.52	0.42
1:A:834:LYS:HE2	2:B:24:GLU:CD	2.44	0.42
2:B:20:LYS:NZ	2:B:20:LYS:HB3	2.35	0.42
3:C:43:ASN:H	3:C:80:GLN:NE2	2.18	0.42
3:C:67:GLU:C	3:C:70:PRO:HD2	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:71:PRO:CG	2:E:76:MET:HE1	2.50	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:135:LYS:HB2	2:E:135:LYS:NZ	2.36	0.41
2:B:59:LYS:HA	2:B:59:LYS:HD2	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:HA	2:E:36:ARG:HD3	1.96	0.41
2:E:54:ARG:H	2:E:54:ARG:HG3	1.65	0.40
2:E:66:LYS:C	2:E:68:ALA:N	2.78	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:C:22:ASP:O	3:C:22:ASP:CG	2.64	0.40
3:F:9:ASP:HB3	6:F:463:HOH:O	2.21	0.40
2:B:22:MET:CE	6:B:766:HOH:O	2.67	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 [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	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%)	5	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	30	31

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%)	58 (92%)	5 (8%)	11	9
1	D	64/64 (100%)	58 (91%)	6 (9%)	8	6
2	B	126/140 (90%)	114 (90%)	12 (10%)	8	6
2	E	129/140 (92%)	110 (85%)	19 (15%)	3	1
3	C	129/133 (97%)	117 (91%)	12 (9%)	8	6
3	F	128/133 (96%)	124 (97%)	4 (3%)	35	44
All	All	639/674 (95%)	581 (91%)	58 (9%)	9	7

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	770	LEU
1	A	779	SER
1	A	788	HIS
1	A	793	LEU
1	A	821	LEU
2	B	17	LEU
2	B	22	MET

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Mol	Chain	Res	Type
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	49	VAL
3	C	95	ARG
3	C	101	ILE
3	C	109	VAL
3	C	132	GLN
3	C	135	LEU
3	C	136	GLU
3	C	153	TYR
1	D	770	LEU
1	D	772	GLU
1	D	788	HIS
1	D	805	ARG
1	D	817	LYS
1	D	822	ARG
2	E	12	ASN
2	E	16	ARG
2	E	19	GLN
2	E	40	ILE
2	E	41	ASP
2	E	42	ILE
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

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Mol	Chain	Res	Type
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	825	GLN
2	B	19	GLN
2	B	34	GLN
2	B	35	ASN
2	B	96	ASN
3	C	5	GLN
3	C	56	HIS
3	C	108	HIS
3	C	132	GLN
3	C	138	ASN
2	E	19	GLN
2	E	23	GLN
2	E	43	ASN
2	E	73	ASN
2	E	96	ASN
2	E	120	ASN
3	F	5	GLN
3	F	80	GLN
3	F	132	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 [i](#)

There are no oligosaccharides 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%)	-0.03	2 (2%) 53 54	25, 34, 54, 66	0
1	D	69/69 (100%)	0.08	1 (1%) 73 74	20, 39, 75, 82	0
2	B	141/161 (87%)	0.08	6 (4%) 40 39	20, 37, 58, 74	0
2	E	145/161 (90%)	0.62	13 (8%) 15 14	20, 49, 81, 92	0
3	C	152/156 (97%)	-0.06	2 (1%) 75 76	25, 37, 57, 68	0
3	F	151/156 (96%)	0.25	5 (3%) 49 49	20, 45, 84, 98	0
All	All	726/772 (94%)	0.18	29 (3%) 42 42	20, 40, 74, 98	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	69	PRO	7.4
2	B	16	ARG	7.0
2	E	156	SER	5.3
2	E	68	ALA	4.9
2	B	17	LEU	4.4
3	F	135	LEU	4.3
1	A	770	LEU	4.2
2	E	70	GLY	3.8
2	E	155	GLY	3.5
2	B	156	SER	3.3
3	F	26	GLY	3.2
1	A	837	LEU	3.2
3	C	21	TRP	3.0
2	E	76	MET	3.0
3	F	150	THR	2.9
2	B	155	GLY	2.8
2	E	40	ILE	2.7
2	E	42	ILE	2.5
2	B	73	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	770	LEU	2.4
3	F	96	GLU	2.4
2	E	12	ASN	2.3
3	C	153	TYR	2.2
3	F	95	ARG	2.1
2	E	54	ARG	2.1
2	E	15	ALA	2.1
2	E	22	MET	2.0
2	B	37	ASP	2.0
2	E	17	LEU	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](#)

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(Å ²)	Q<0.9
4	MG	B	162	1/1	0.85	0.17	44,44,44,44	0
4	MG	E	162	1/1	0.94	0.12	67,67,67,67	0
5	CA	C	157	1/1	0.94	0.05	46,46,46,46	0
5	CA	F	157	1/1	0.99	0.03	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.