



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2020 – 04:03 PM BST

PDB ID : 6ZN3
Title : Plasmodium falciparum glideosome trimeric sub-complex
Authors : Pazicky, S.; Loew, C.
Deposited on : 2020-07-06
Resolution : 2.51 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 : 2.14.6
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) : 2.14.6

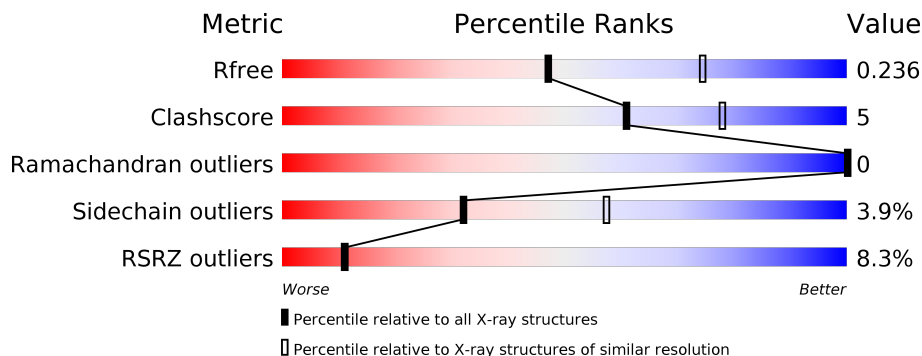
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	135	
1	D	135	
1	G	135	
1	J	135	
1	M	135	
2	B	147	

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Mol	Chain	Length	Quality of chain
2	E	147	<p>3% 86% 10% . .</p>
2	H	147	<p>5% 87% 7% . 5%</p>
2	K	147	<p>7% 86% 11% .</p>
2	N	147	<p>3% 82% 12% . 5%</p>
3	C	43	<p>2% 88% 12%</p>
3	F	43	<p>2% 81% 16% .</p>
3	I	43	<p>79% 21%</p>
3	L	43	<p>81% 16% .</p>
3	O	43	<p>79% 19% .</p>

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 12968 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 essential light chain ELC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	135	1106	703	180	216	7	0	0	0
1	D	135	1106	703	180	216	7	0	0	0
1	G	135	1106	703	180	216	7	0	0	0
1	J	135	1106	703	180	216	7	0	0	0
1	M	135	1106	703	180	216	7	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q8IJM4
D	0	SER	-	expression tag	UNP Q8IJM4
G	0	SER	-	expression tag	UNP Q8IJM4
J	0	SER	-	expression tag	UNP Q8IJM4
M	0	SER	-	expression tag	UNP Q8IJM4

- Molecule 2 is a protein called Myosin A tail domain interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	140	1127	708	179	235	5	0	0	0
2	E	143	1147	720	182	240	5	0	0	0
2	H	140	1127	708	179	235	5	0	0	0
2	K	143	1147	720	182	240	5	0	0	0
2	N	140	1127	708	179	235	5	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	58	SER	-	expression tag	UNP Q8I4W8
B	59	MET	-	expression tag	UNP Q8I4W8
E	58	SER	-	expression tag	UNP Q8I4W8
E	59	MET	-	expression tag	UNP Q8I4W8
H	58	SER	-	expression tag	UNP Q8I4W8
H	59	MET	-	expression tag	UNP Q8I4W8
K	58	SER	-	expression tag	UNP Q8I4W8
K	59	MET	-	expression tag	UNP Q8I4W8
N	58	SER	-	expression tag	UNP Q8I4W8
N	59	MET	-	expression tag	UNP Q8I4W8

- Molecule 3 is a protein called Myosin-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	43	Total	C	N	O	S	0	0	0
			352	226	66	58	2			
3	F	43	Total	C	N	O	S	0	0	0
			352	226	66	58	2			
3	I	43	Total	C	N	O	S	0	0	0
			352	226	66	58	2			
3	L	43	Total	C	N	O	S	0	0	0
			352	226	66	58	2			
3	O	43	Total	C	N	O	S	0	0	0
			352	226	66	58	2			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	774	SER	-	expression tag	UNP Q8IDR3
F	774	SER	-	expression tag	UNP Q8IDR3
I	774	SER	-	expression tag	UNP Q8IDR3
L	774	SER	-	expression tag	UNP Q8IDR3
O	774	SER	-	expression tag	UNP Q8IDR3

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	O	0	0
			1	1		
4	J	1	Total	O	0	0
			1	1		

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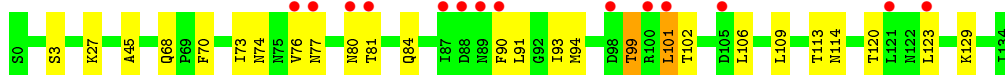
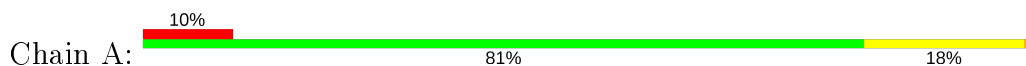
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	N	1	Total	O	0	0
			1	1		

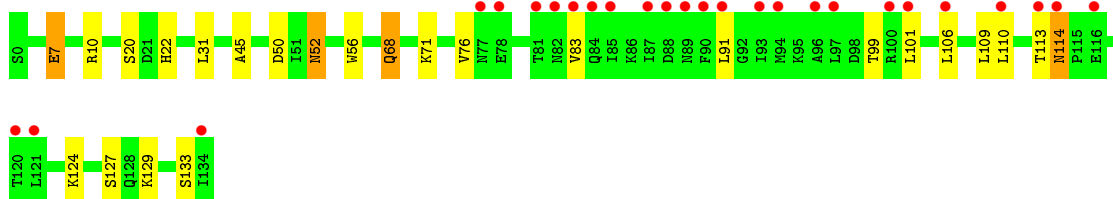
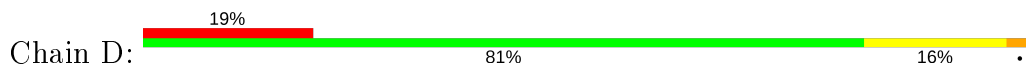
3 Residue-property plots [i](#)

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.

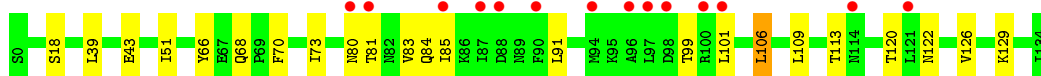
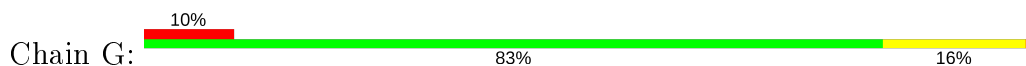
- Molecule 1: Myosin essential light chain ELC



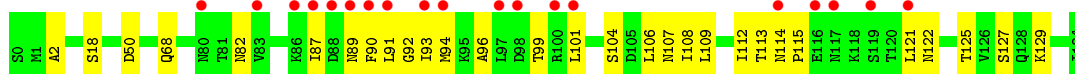
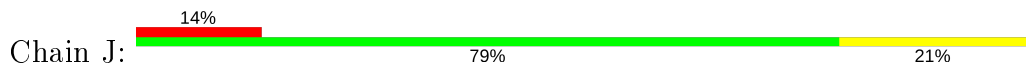
- Molecule 1: Myosin essential light chain ELC



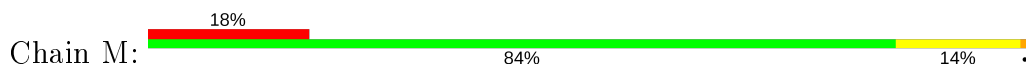
- Molecule 1: Myosin essential light chain ELC

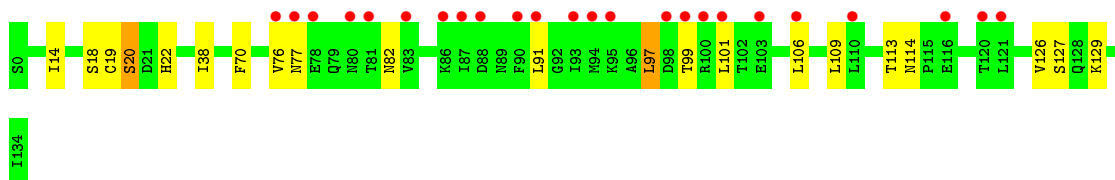


- Molecule 1: Myosin essential light chain ELC

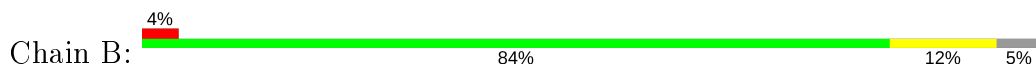


- Molecule 1: Myosin essential light chain ELC

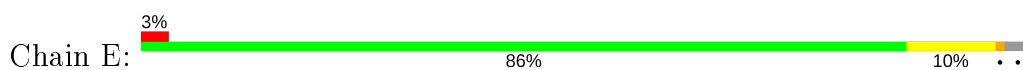




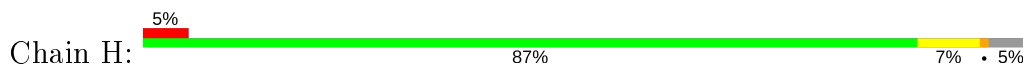
- Molecule 2: Myosin A tail domain interacting protein



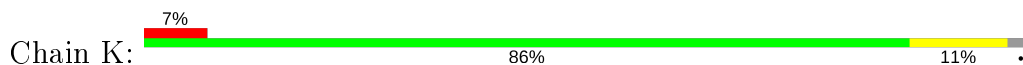
- Molecule 2: Myosin A tail domain interacting protein



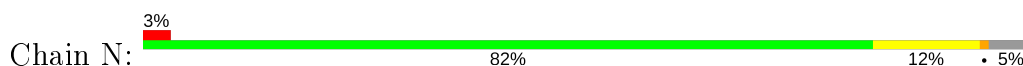
- Molecule 2: Myosin A tail domain interacting protein



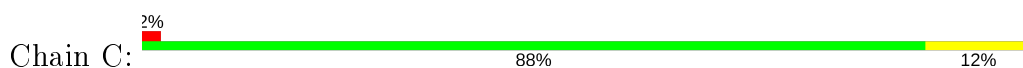
- Molecule 2: Myosin A tail domain interacting protein



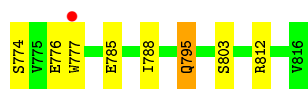
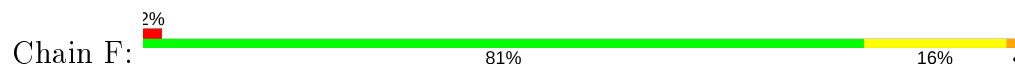
- Molecule 2: Myosin A tail domain interacting protein



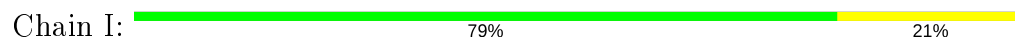
- Molecule 3: Myosin-A



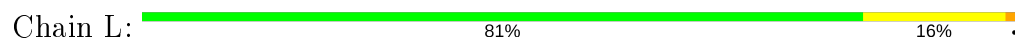
- Molecule 3: Myosin-A



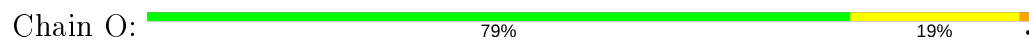
- Molecule 3: Myosin-A



- Molecule 3: Myosin-A



- Molecule 3: Myosin-A



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	211.88Å 211.88Å 75.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.42 – 2.51 47.38 – 2.51	Depositor EDS
% Data completeness (in resolution range)	83.5 (47.42-2.51) 83.6 (47.38-2.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.8.0258, PHENIX 1.17.1.3660	Depositor
R, R_{free}	0.200 , 0.238 0.203 , 0.236	Depositor DCC
R_{free} test set	4756 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	81.4	Xtrriage
Anisotropy	0.026	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12968	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.75	0/1126	0.89	0/1518
1	D	0.75	0/1126	0.92	1/1518 (0.1%)
1	G	0.76	0/1126	0.89	0/1518
1	J	0.77	0/1126	0.86	0/1518
1	M	0.75	0/1126	0.87	1/1518 (0.1%)
2	B	0.76	0/1144	0.91	1/1542 (0.1%)
2	E	0.73	0/1164	0.93	2/1570 (0.1%)
2	H	0.73	0/1144	0.91	0/1542
2	K	0.75	0/1164	0.91	0/1570
2	N	0.76	0/1144	0.89	0/1542
3	C	0.70	0/357	0.97	1/478 (0.2%)
3	F	0.67	0/357	0.98	1/478 (0.2%)
3	I	0.67	0/357	1.03	0/478
3	L	0.66	0/357	0.95	1/478 (0.2%)
3	O	0.68	0/357	1.04	1/478 (0.2%)
All	All	0.74	0/13175	0.91	9/17746 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	2
1	J	0	1
1	M	0	1
All	All	0	5

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	78	ARG	CB-CA-C	8.99	128.38	110.40
1	D	7	GLU	CB-CA-C	6.20	122.81	110.40
3	C	795	GLN	CB-CA-C	5.61	121.62	110.40
3	F	795	GLN	CB-CA-C	5.61	121.61	110.40
1	M	20	SER	N-CA-CB	5.40	118.60	110.50
3	O	795	GLN	CB-CA-C	5.27	120.94	110.40
2	E	78	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	B	110	ASP	CB-CA-C	5.08	120.56	110.40
3	L	795	GLN	CB-CA-C	5.06	120.52	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	ASN	Peptide
1	D	114	ASN	Peptide
1	D	133	SER	Peptide
1	J	114	ASN	Peptide
1	M	114	ASN	Peptide

5.2 Too-close contacts [i](#)

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	1106	0	1088	18	0
1	D	1106	0	1088	16	0
1	G	1106	0	1088	11	0
1	J	1106	0	1088	16	0
1	M	1106	0	1088	10	0
2	B	1127	0	1081	9	0
2	E	1147	0	1099	8	0
2	H	1127	0	1081	6	0
2	K	1147	0	1099	8	0
2	N	1127	0	1081	9	0
3	C	352	0	383	5	0
3	F	352	0	383	7	0
3	I	352	0	383	6	0
3	L	352	0	383	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	352	0	383	8	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
4	N	1	0	0	0	0
All	All	12968	0	12796	117	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 5.

All (117) 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:D:76:VAL:HG12	3:F:776:GLU:HB3	1.45	0.98
2:E:115:LYS:HE2	2:E:120:ASP:OD1	1.90	0.71
2:K:115:LYS:HE2	2:K:120:ASP:OD1	1.89	0.71
1:J:91:LEU:HD22	1:J:106:LEU:HD21	1.76	0.68
1:J:109:LEU:HD13	3:L:788:ILE:HD11	1.76	0.67
1:D:109:LEU:HD13	3:F:788:ILE:HD11	1.75	0.67
2:N:154:ASN:HB2	2:N:156:THR:HG23	1.75	0.67
1:M:109:LEU:HD13	3:O:788:ILE:HD11	1.78	0.66
1:D:76:VAL:CG1	3:F:776:GLU:HB3	2.23	0.65
1:M:101:LEU:HD11	3:O:785:GLU:HA	1.79	0.65
1:D:76:VAL:HG12	3:F:776:GLU:CB	2.26	0.64
1:M:14:ILE:HG23	1:M:19:CYS:SG	2.37	0.64
2:B:148:PHE:CE1	2:B:164:MET:CE	2.83	0.61
1:A:99:THR:HB	1:A:101:LEU:HD12	1.83	0.61
2:B:96:SER:O	2:B:100:ARG:HG3	2.00	0.61
1:M:20:SER:HB3	1:M:22:HIS:H	1.65	0.60
3:I:798:ASN:HA	3:I:801:ILE:HD12	1.84	0.59
2:K:96:SER:O	2:K:100:ARG:HG3	2.03	0.58
1:A:74:ASN:HA	1:A:77:ASN:HD22	1.69	0.58
2:N:67:GLN:NE2	2:N:137:ASP:OD2	2.38	0.57
1:D:91:LEU:HD13	1:D:106:LEU:HD22	1.86	0.56
1:A:91:LEU:HD13	1:A:106:LEU:HD22	1.88	0.56
2:E:96:SER:O	2:E:100:ARG:HG3	2.06	0.56
1:A:77:ASN:HA	1:A:80:ASN:O	2.07	0.55
1:D:68:GLN:NE2	1:D:71:LYS:HG3	2.21	0.55
1:A:76:VAL:HG21	3:C:780:CYS:HB2	1.89	0.55
2:H:154:ASN:HB2	2:H:156:THR:HG23	1.88	0.55
2:E:173:ASP:O	3:F:812:ARG:NH2	2.40	0.54
1:A:113:THR:HA	1:A:129:LYS:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:90:PHE:O	1:J:94:MET:HG2	2.08	0.54
2:K:67:GLN:O	2:K:71:LYS:HG2	2.07	0.53
2:B:115:LYS:HE2	2:B:120:ASP:OD1	2.07	0.53
1:A:27:LYS:NZ	3:C:793:TYR:OH	2.41	0.53
2:N:96:SER:O	2:N:100:ARG:HG3	2.08	0.53
1:G:91:LEU:HD13	1:G:106:LEU:HD22	1.91	0.53
2:N:160:THR:OG1	2:N:163:GLN:HG3	2.10	0.51
2:B:160:THR:OG1	2:B:163:GLN:HG3	2.10	0.50
1:D:45:ALA:HB1	1:J:2:ALA:HB2	1.94	0.49
2:E:67:GLN:O	2:E:71:LYS:HG2	2.11	0.49
1:G:109:LEU:HD13	3:I:788:ILE:HD11	1.93	0.49
1:M:91:LEU:HD13	1:M:106:LEU:HD22	1.93	0.49
1:D:106:LEU:O	1:D:109:LEU:HB3	2.13	0.49
2:H:106:PRO:HB3	2:H:134:CYS:SG	2.53	0.49
1:M:18:SER:CB	2:N:153:ASN:HD21	2.26	0.48
1:A:84:GLN:HB3	1:A:120:THR:HB	1.96	0.48
2:E:176:THR:HG23	2:E:179:GLU:OE1	2.14	0.48
1:J:87:ILE:O	1:J:91:LEU:HG	2.13	0.47
2:K:114:ILE:HG12	2:K:130:TYR:HB2	1.96	0.47
1:G:80:ASN:O	1:G:83:VAL:HG13	2.14	0.47
1:J:101:LEU:HD11	3:L:785:GLU:HA	1.96	0.47
1:A:93:ILE:HG21	3:C:777:TRP:CH2	2.50	0.47
2:N:202:ILE:HA	3:O:814:LYS:HD3	1.96	0.47
1:D:101:LEU:HD11	3:F:785:GLU:HA	1.97	0.47
1:G:70:PHE:HB3	1:G:73:ILE:HD12	1.96	0.47
3:I:816:VAL:O	3:I:816:VAL:HG13	2.15	0.47
2:K:202:ILE:HA	3:L:814:LYS:HD3	1.94	0.47
2:N:106:PRO:HB3	2:N:134:CYS:SG	2.54	0.47
1:D:110:LEU:O	1:D:114:ASN:HB2	2.15	0.47
1:J:115:PRO:HD3	1:J:129:LYS:HE3	1.96	0.47
2:K:154:ASN:HB2	2:K:156:THR:HG23	1.95	0.47
3:O:777:TRP:O	3:O:781:VAL:HG13	2.15	0.46
1:J:82:ASN:HB2	1:J:122:ASN:HB2	1.98	0.46
1:J:91:LEU:HD22	1:J:106:LEU:HD11	1.98	0.46
2:B:148:PHE:CD1	2:B:164:MET:CE	2.99	0.46
3:I:801:ILE:N	3:I:802:PRO:HD2	2.30	0.46
1:A:109:LEU:HB2	3:C:788:ILE:HD11	1.97	0.46
1:M:70:PHE:HD1	3:O:783:VAL:CG1	2.29	0.46
2:N:68:LEU:O	2:N:72:VAL:HG22	2.16	0.45
1:A:99:THR:HB	1:A:101:LEU:CD1	2.46	0.45
3:L:798:ASN:HA	3:L:801:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:PHE:CE1	2:B:164:MET:HE3	2.52	0.45
1:D:31:LEU:HD21	1:D:56:TRP:CE2	2.52	0.45
1:M:113:THR:HA	1:M:129:LYS:HG3	1.98	0.45
1:A:101:LEU:O	1:A:101:LEU:HD13	2.16	0.45
1:D:52:ASN:ND2	1:D:52:ASN:H	2.15	0.44
3:O:781:VAL:HG23	3:O:785:GLU:OE2	2.18	0.44
1:G:113:THR:HA	1:G:129:LYS:HG3	1.98	0.44
1:G:101:LEU:HD11	3:I:785:GLU:HA	2.00	0.44
1:J:108:ILE:O	1:J:112:ILE:HG13	2.16	0.44
1:J:113:THR:O	1:J:129:LYS:HG3	2.17	0.44
1:J:91:LEU:HD13	1:J:106:LEU:HD21	1.99	0.44
2:K:69:GLU:HG2	2:K:74:GLU:OE2	2.18	0.43
1:J:92:GLY:O	1:J:96:ALA:HB2	2.17	0.43
1:G:80:ASN:ND2	1:G:85:ILE:HD11	2.34	0.43
2:H:192:ASN:ND2	2:H:192:ASN:N	2.67	0.43
2:N:108:SER:OG	2:N:173:ASP:OD1	2.27	0.43
1:J:113:THR:HA	1:J:129:LYS:HG3	2.00	0.43
1:G:39:LEU:HB3	1:G:43:GLU:HB2	2.01	0.43
2:H:92:ILE:HD12	2:H:114:ILE:HG23	2.01	0.42
1:J:89:ASN:O	1:J:93:ILE:HG13	2.19	0.42
2:H:192:ASN:HD22	2:H:192:ASN:N	2.17	0.42
1:J:104:SER:HA	1:J:107:ASN:HD22	1.84	0.42
2:K:148:PHE:CE1	2:K:164:MET:HE2	2.55	0.42
2:E:152:ASP:OD2	2:E:157:GLY:N	2.51	0.42
2:H:68:LEU:O	2:H:72:VAL:HG22	2.20	0.42
2:B:89:LYS:HA	2:B:122:LEU:O	2.20	0.41
2:B:65:ILE:HG22	2:B:67:GLN:H	1.83	0.41
1:A:45:ALA:HB2	1:G:66:TYR:CE2	2.55	0.41
1:D:20:SER:HB3	1:D:22:HIS:H	1.85	0.41
1:A:76:VAL:CG2	3:C:780:CYS:HB2	2.50	0.41
1:G:113:THR:O	1:G:129:LYS:HG3	2.19	0.41
1:A:90:PHE:O	1:A:94:MET:HG2	2.20	0.41
1:M:97:LEU:HA	1:M:97:LEU:HD13	1.88	0.41
1:G:84:GLN:HB3	1:G:120:THR:HB	2.01	0.41
1:M:70:PHE:CD1	3:O:783:VAL:CG1	3.03	0.41
1:D:124:LYS:HB3	1:D:124:LYS:HE2	1.94	0.41
1:D:91:LEU:O	1:D:91:LEU:HD12	2.21	0.41
2:E:108:SER:OG	2:E:173:ASP:OD1	2.26	0.41
3:O:789:LEU:HD12	3:O:789:LEU:HA	1.91	0.41
1:A:77:ASN:HD21	1:A:123:LEU:HB2	1.86	0.41
3:F:774:SER:HB3	3:F:777:TRP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PHE:HB3	1:A:73:ILE:HD12	2.03	0.40
1:A:77:ASN:O	1:A:81:THR:HA	2.21	0.40
2:B:92:ILE:HD12	2:B:114:ILE:CG2	2.51	0.40
1:D:113:THR:HA	1:D:129:LYS:HG3	2.03	0.40
3:I:789:LEU:HA	3:I:789:LEU:HD12	1.81	0.40
2:E:148:PHE:CE1	2:E:164:MET:HE2	2.57	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	133/135 (98%)	126 (95%)	7 (5%)	0	100	100
1	D	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
1	G	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
1	J	133/135 (98%)	129 (97%)	4 (3%)	0	100	100
1	M	133/135 (98%)	127 (96%)	6 (4%)	0	100	100
2	B	138/147 (94%)	136 (99%)	2 (1%)	0	100	100
2	E	141/147 (96%)	139 (99%)	2 (1%)	0	100	100
2	H	138/147 (94%)	135 (98%)	3 (2%)	0	100	100
2	K	141/147 (96%)	136 (96%)	5 (4%)	0	100	100
2	N	138/147 (94%)	136 (99%)	2 (1%)	0	100	100
3	C	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
3	F	41/43 (95%)	41 (100%)	0	0	100	100
3	I	41/43 (95%)	41 (100%)	0	0	100	100
3	L	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
3	O	41/43 (95%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1566/1625 (96%)	1525 (97%)	41 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	127/127 (100%)	122 (96%)	5 (4%)	32	57
1	D	127/127 (100%)	119 (94%)	8 (6%)	18	34
1	G	127/127 (100%)	119 (94%)	8 (6%)	18	34
1	J	127/127 (100%)	120 (94%)	7 (6%)	21	41
1	M	127/127 (100%)	119 (94%)	8 (6%)	18	34
2	B	126/132 (96%)	124 (98%)	2 (2%)	62	84
2	E	128/132 (97%)	126 (98%)	2 (2%)	62	84
2	H	126/132 (96%)	122 (97%)	4 (3%)	39	65
2	K	128/132 (97%)	127 (99%)	1 (1%)	81	93
2	N	126/132 (96%)	122 (97%)	4 (3%)	39	65
3	C	40/40 (100%)	40 (100%)	0	100	100
3	F	40/40 (100%)	38 (95%)	2 (5%)	24	46
3	I	40/40 (100%)	38 (95%)	2 (5%)	24	46
3	L	40/40 (100%)	37 (92%)	3 (8%)	13	26
3	O	40/40 (100%)	38 (95%)	2 (5%)	24	46
All	All	1469/1495 (98%)	1411 (96%)	58 (4%)	32	57

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

Mol	Chain	Res	Type
1	A	3	SER
1	A	68	GLN

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Mol	Chain	Res	Type
1	A	99	THR
1	A	101	LEU
1	A	102	THR
2	B	133	ILE
2	B	144	LEU
1	D	7	GLU
1	D	10	ARG
1	D	50	ASP
1	D	52	ASN
1	D	68	GLN
1	D	83	VAL
1	D	99	THR
1	D	127	SER
2	E	78	ARG
2	E	133	ILE
3	F	795	GLN
3	F	803	SER
1	G	18	SER
1	G	51	ILE
1	G	68	GLN
1	G	81	THR
1	G	99	THR
1	G	106	LEU
1	G	122	ASN
1	G	126	VAL
2	H	113	LYS
2	H	133	ILE
2	H	154	ASN
2	H	177	ASP
3	I	803	SER
3	I	814	LYS
1	J	18	SER
1	J	50	ASP
1	J	68	GLN
1	J	99	THR
1	J	121	LEU
1	J	125	THR
1	J	127	SER
2	K	144	LEU
3	L	782	SER
3	L	803	SER
3	L	814	LYS

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Mol	Chain	Res	Type
1	M	38	ILE
1	M	76	VAL
1	M	77	ASN
1	M	82	ASN
1	M	97	LEU
1	M	99	THR
1	M	126	VAL
1	M	127	SER
2	N	113	LYS
2	N	133	ILE
2	N	154	ASN
2	N	204	GLN
3	O	795	GLN
3	O	803	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	D	52	ASN
1	G	77	ASN
1	G	117	ASN
1	G	122	ASN
2	H	192	ASN
1	J	68	GLN
1	J	74	ASN
1	J	77	ASN
1	J	84	GLN
1	J	107	ASN
2	K	192	ASN
2	N	153	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 monosaccharides 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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	135/135 (100%)	0.58	14 (10%) 6 6	52, 86, 187, 207	3 (2%)
1	D	135/135 (100%)	1.03	26 (19%) 1 1	60, 91, 196, 230	3 (2%)
1	G	135/135 (100%)	0.54	14 (10%) 6 6	52, 90, 202, 230	3 (2%)
1	J	135/135 (100%)	0.64	19 (14%) 2 2	55, 91, 192, 213	3 (2%)
1	M	135/135 (100%)	0.90	24 (17%) 1 1	58, 83, 200, 248	3 (2%)
2	B	140/147 (95%)	0.07	6 (4%) 35 38	61, 81, 124, 187	1 (0%)
2	E	143/147 (97%)	0.19	4 (2%) 53 56	64, 92, 142, 197	1 (0%)
2	H	140/147 (95%)	0.17	8 (5%) 23 25	67, 93, 168, 188	1 (0%)
2	K	143/147 (97%)	0.36	11 (7%) 13 13	67, 93, 165, 186	1 (0%)
2	N	140/147 (95%)	0.15	5 (3%) 42 46	62, 89, 132, 168	1 (0%)
3	C	43/43 (100%)	0.42	1 (2%) 60 63	59, 70, 103, 120	0
3	F	43/43 (100%)	0.38	1 (2%) 60 63	66, 85, 121, 137	0
3	I	43/43 (100%)	0.33	0 100 100	59, 77, 107, 122	0
3	L	43/43 (100%)	0.36	0 100 100	59, 74, 112, 124	0
3	O	43/43 (100%)	0.36	0 100 100	64, 77, 108, 119	0
All	All	1596/1625 (98%)	0.44	133 (8%) 11 11	52, 88, 183, 248	20 (1%)

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	121	LEU	8.2
1	M	94	MET	7.5
1	M	101	LEU	7.1
1	M	90	PHE	6.8
2	B	68	LEU	6.6
1	D	87	ILE	6.3
2	K	64	ASP	6.3

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Mol	Chain	Res	Type	RSRZ
1	M	88	ASP	5.8
1	D	93	ILE	5.5
1	D	94	MET	5.4
2	K	65	ILE	5.4
2	K	72	VAL	5.3
1	M	81	THR	5.1
1	D	90	PHE	5.0
1	A	90	PHE	4.9
2	K	68	LEU	4.8
1	D	81	THR	4.8
2	H	66	GLN	4.7
2	H	68	LEU	4.6
1	M	87	ILE	4.6
2	N	66	GLN	4.6
1	J	87	ILE	4.6
2	B	67	GLN	4.6
1	G	90	PHE	4.5
1	M	120	THR	4.4
2	N	71	LYS	4.4
2	N	67	GLN	4.4
1	J	101	LEU	4.4
1	D	82	ASN	4.4
1	D	134	ILE	4.4
1	M	77	ASN	4.3
1	M	121	LEU	4.3
1	D	88	ASP	4.2
1	J	91	LEU	4.2
1	A	101	LEU	4.2
2	K	69	GLU	4.1
1	G	81	THR	4.1
1	J	80	ASN	4.0
2	K	66	GLN	4.0
1	A	81	THR	4.0
1	M	100	ARG	3.9
1	A	77	ASN	3.8
2	K	62	VAL	3.8
1	J	90	PHE	3.8
1	G	87	ILE	3.8
2	K	63	ALA	3.8
1	J	100	ARG	3.8
1	G	121	LEU	3.8
1	M	80	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	88	ASP	3.7
1	D	101	LEU	3.7
1	A	98	ASP	3.7
1	G	80	ASN	3.6
1	A	80	ASN	3.6
1	A	87	ILE	3.6
1	D	83	VAL	3.6
1	G	94	MET	3.5
1	J	114	ASN	3.5
1	M	98	ASP	3.4
1	J	83	VAL	3.4
1	D	120	THR	3.4
1	D	89	ASN	3.3
1	D	91	LEU	3.3
2	B	66	GLN	3.3
1	J	116	GLU	3.2
3	F	777	TRP	3.2
2	E	64	ASP	3.1
1	D	84	GLN	3.1
2	K	67	GLN	3.1
1	A	100	ARG	3.1
1	G	96	ALA	3.1
2	K	71	LYS	3.1
1	D	78	GLU	3.0
1	G	85	ILE	3.0
2	K	70	GLU	3.0
1	G	101	LEU	3.0
3	C	777	TRP	3.0
1	A	88	ASP	2.9
1	D	77	ASN	2.9
1	A	123	LEU	2.9
2	H	67	GLN	2.9
1	G	100	ARG	2.8
1	D	85	ILE	2.8
2	H	71	LYS	2.7
2	N	68	LEU	2.7
1	A	76	VAL	2.7
1	M	95	LYS	2.7
1	J	97	LEU	2.7
1	M	110	LEU	2.6
2	E	67	GLN	2.6
2	H	70	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	62	VAL	2.6
1	D	100	ARG	2.6
1	J	86	LYS	2.6
1	M	116	GLU	2.5
1	J	119	SER	2.5
1	D	96	ALA	2.5
1	A	89	ASN	2.5
1	J	121	LEU	2.5
2	B	69	GLU	2.4
2	B	71	LYS	2.4
2	H	69	GLU	2.4
2	E	63	ALA	2.4
1	J	93	ILE	2.3
1	M	106	LEU	2.3
1	D	106	LEU	2.3
2	B	72	VAL	2.3
1	D	116	GLU	2.3
1	D	113	THR	2.3
1	A	121	LEU	2.2
1	M	91	LEU	2.2
1	J	89	ASN	2.2
1	M	83	VAL	2.2
1	J	88	ASP	2.1
1	D	97	LEU	2.1
1	D	110	LEU	2.1
1	G	97	LEU	2.1
1	G	114	ASN	2.1
1	M	76	VAL	2.1
2	H	114	ILE	2.1
1	G	98	ASP	2.1
2	H	65	ILE	2.1
1	M	99	THR	2.1
1	M	86	LYS	2.1
1	J	94	MET	2.1
1	A	105	ASP	2.1
1	M	93	ILE	2.1
1	J	117	ASN	2.1
1	J	98	ASP	2.0
1	M	103	GLU	2.0
1	D	114	ASN	2.0
2	N	72	VAL	2.0
1	M	78	GLU	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 monosaccharides 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.