W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Mar 21, 2016 – 12:32 PM EDT

PDB ID	:	5FJY
Title	:	Crystal structure of mouse kinesin light chain 2 (residues 161-480)
Authors	:	Pernigo, S.; Yip, Y.Y.; Sanger, A.; Xu, M.; Dodding, M.P.; Steiner, R.A.
Deposited on	:	2015-10-14
Resolution	:	4.00 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

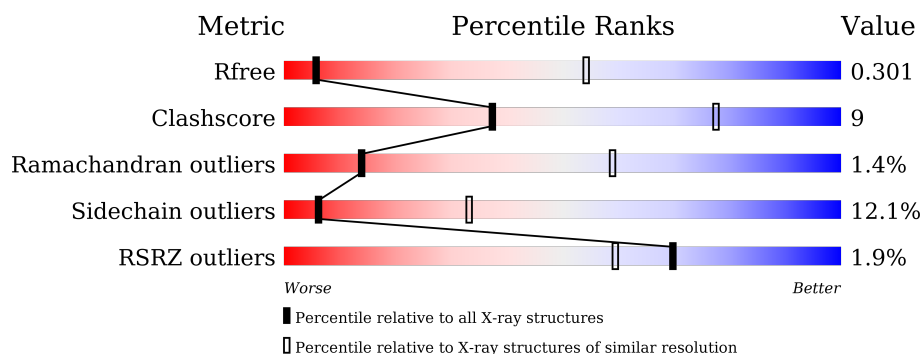|		
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 4.00 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	Percentile Ranks	Value
Rfree		0.301
Clashscore		9
Ramachandran outliers		1.4%
Sidechain outliers		12.1%
RSRZ outliers		1.9%

Worse ← → *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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. 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	324	%　63%　18%　•　18%
1	B	324	%　55%　23%　•　18%
1	C	324	3%　61%　18%　•　18%
2	D	5	80%　20%
2	E	5	80%　20%
2	F	5	40%　60%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6405 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 KINESIN LIGHT CHAIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2115	1323	384	400	8			
1	B	267	Total	C	N	O	S	0	0	0
			2115	1323	384	400	8			
1	C	267	Total	C	N	O	S	0	0	0
			2115	1323	384	400	8			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	157	GLY	-	EXPRESSION TAG	UNP Q91YS4
A	158	SER	-	EXPRESSION TAG	UNP Q91YS4
A	159	HIS	-	EXPRESSION TAG	UNP Q91YS4
A	160	MET	-	EXPRESSION TAG	UNP Q91YS4
A	197	LEU	ARG	CONFLICT	UNP Q91YS4
A	198	ARG	LEU	CONFLICT	UNP Q91YS4
A	199	LEU	ARG	CONFLICT	UNP Q91YS4
B	157	GLY	-	EXPRESSION TAG	UNP Q91YS4
B	158	SER	-	EXPRESSION TAG	UNP Q91YS4
B	159	HIS	-	EXPRESSION TAG	UNP Q91YS4
B	160	MET	-	EXPRESSION TAG	UNP Q91YS4
B	197	LEU	ARG	CONFLICT	UNP Q91YS4
B	198	ARG	LEU	CONFLICT	UNP Q91YS4
B	199	LEU	ARG	CONFLICT	UNP Q91YS4
C	157	GLY	-	EXPRESSION TAG	UNP Q91YS4
C	158	SER	-	EXPRESSION TAG	UNP Q91YS4
C	159	HIS	-	EXPRESSION TAG	UNP Q91YS4
C	160	MET	-	EXPRESSION TAG	UNP Q91YS4
C	197	LEU	ARG	CONFLICT	UNP Q91YS4
C	198	ARG	LEU	CONFLICT	UNP Q91YS4
C	199	LEU	ARG	CONFLICT	UNP Q91YS4

- Molecule 2 is a protein called UNKNOWN PEPTIDE.

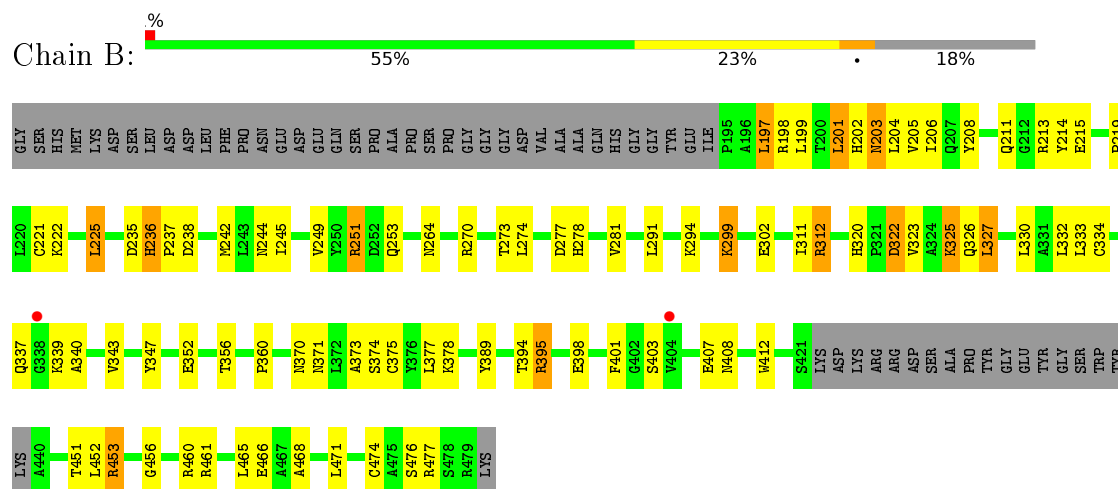| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	5	Total 25	C 15	N 5	O 5	0	0	0
2	E	5	Total 25	C 15	N 5	O 5	0	0	0
2	F	2	Total 10	C 6	N 2	O 2	0	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: KINESIN LIGHT CHAIN 2
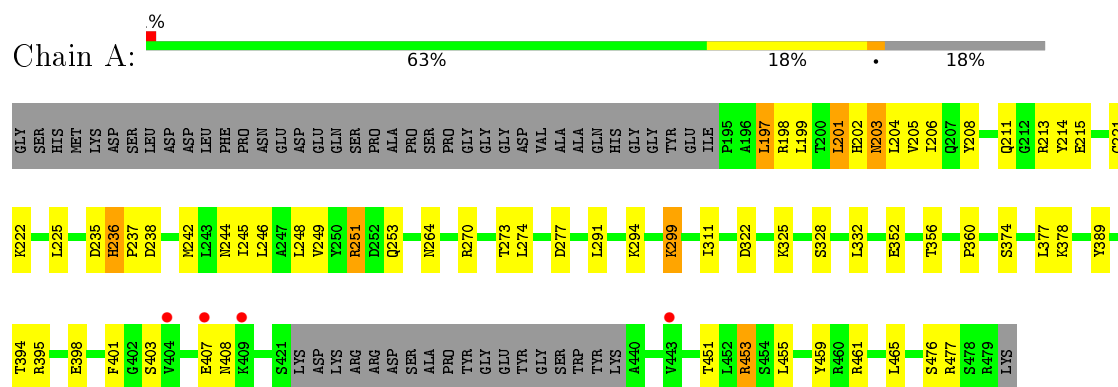
- Molecule 1: KINESIN LIGHT CHAIN 2

- Molecule 1: KINESIN LIGHT CHAIN 2

Y347 E352 P360 N371 C375 K378 Y389 R395 E398 F401 G402 S403 E407 N408 R418 S421 LYS ASP LYS ARG ARG ASP SER ALA PRO TYR GLY GLU TYR GLY SER TRP TYR LYS A440 T451 L452 R453 S454 L455 L465 H469 T470 L471 E472

A475 S476 R477 S478 R479 LYS

• Molecule 2: UNKNOWN PEPTIDE

Chain D:

80%   20%

X1001 X1005

• Molecule 2: UNKNOWN PEPTIDE

Chain E:

80%   20%

X1001 X1002 X1005

• Molecule 2: UNKNOWN PEPTIDE

Chain F:

40%   60%

X1001 X1002 UNK UNK
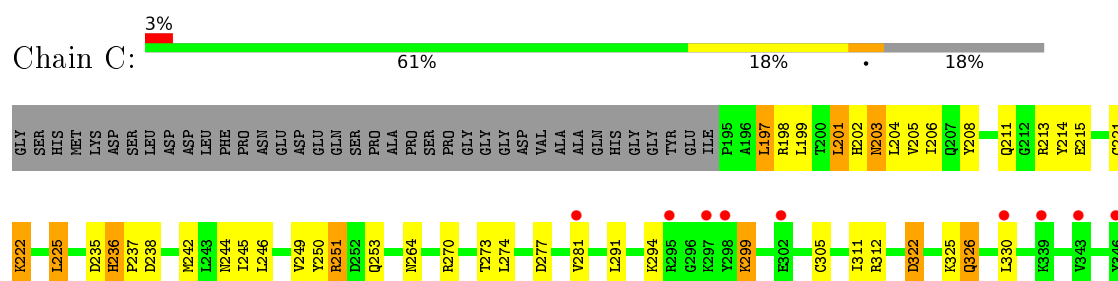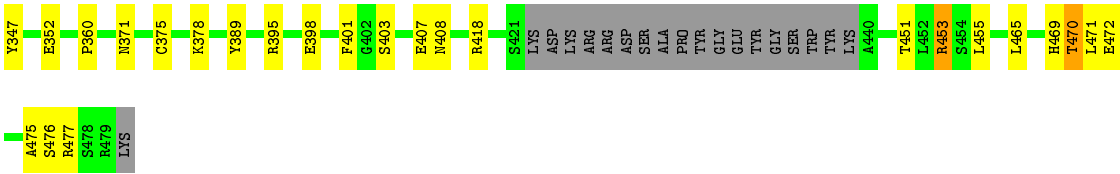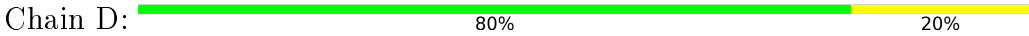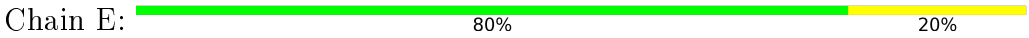
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	148.70Å 86.28Å 111.74Å 90.00° 98.41° 90.00°	Depositor
Resolution (Å)	42.88 – 4.00 42.88 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (42.88-4.00) 98.3 (42.88-4.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 4.00Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.233 , 0.261 0.272 , 0.301	Depositor DCC
R_{free} test set	543 reflections (4.61%)	DCC
Wilson B-factor (Å^2)	177.4	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 224.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.36, < L^2 > = 0.20$	Xtriage
Outliers	0 of 11801 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6405	wwPDB-VP
Average B, all atoms (Å^2)	266.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.50	0/2150	0.66	1/2901 (0.0%)
1	B	0.54	0/2150	0.75	1/2901 (0.0%)
1	C	0.48	0/2150	0.70	1/2901 (0.0%)
All	All	0.51	0/6450	0.70	3/8703 (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	C	235	ASP	C-N-CA	5.22	134.75	121.70
1	A	235	ASP	C-N-CA	5.11	134.48	121.70
1	B	235	ASP	C-N-CA	5.10	134.44	121.70

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	2115	0	2129	36	0
1	B	2115	0	2129	50	0
1	C	2115	0	2129	36	0
2	D	25	0	9	1	0
2	E	25	0	8	1	0
2	F	10	0	4	0	0
All	All	6405	0	6408	119	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 9.

All (119) 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:B:332:LEU:HG	1:B:347:TYR:OH	1.68	0.94
1:B:334:CYS:HB2	1:B:343:VAL:CG2	2.07	0.85
1:A:198:ARG:HG3	1:A:199:LEU:H	1.44	0.82
1:B:198:ARG:HG3	1:B:199:LEU:H	1.44	0.81
1:C:198:ARG:HG3	1:C:199:LEU:H	1.43	0.81
1:B:202:HIS:HB3	1:B:225:LEU:HD21	1.71	0.72
1:A:202:HIS:HB3	1:A:225:LEU:HD21	1.71	0.71
1:C:312:ARG:HD3	1:C:326:GLN:HE21	1.55	0.71
1:C:215:GLU:HG2	1:C:249:VAL:HG13	1.75	0.69
1:A:215:GLU:HG2	1:A:249:VAL:HG13	1.73	0.69
1:C:202:HIS:HB3	1:C:225:LEU:HD21	1.75	0.68
1:B:215:GLU:HG2	1:B:249:VAL:HG13	1.76	0.68
1:A:222:LYS:HZ2	1:A:246:LEU:HD12	1.58	0.68
1:A:360:PRO:HB2	1:A:395:ARG:HD3	1.77	0.65
1:A:199:LEU:HD13	1:A:225:LEU:HD13	1.77	0.65
1:C:198:ARG:HG3	1:C:199:LEU:N	2.12	0.64
1:B:199:LEU:HD13	1:B:225:LEU:HD13	1.79	0.64
1:C:199:LEU:HD13	1:C:225:LEU:HD13	1.80	0.64
1:A:251:ARG:HB2	1:A:291:LEU:HD21	1.78	0.64
1:B:198:ARG:HG3	1:B:199:LEU:N	2.12	0.64
1:B:334:CYS:HB3	1:B:339:LYS:HB2	1.80	0.63
1:A:198:ARG:HG3	1:A:199:LEU:N	2.13	0.63
1:B:360:PRO:HB2	1:B:395:ARG:HD3	1.79	0.63
1:B:334:CYS:HB2	1:B:343:VAL:HG21	1.79	0.63
1:C:360:PRO:HB2	1:C:395:ARG:HD3	1.80	0.62
1:C:251:ARG:HB2	1:C:291:LEU:HD21	1.80	0.62
1:A:236:HIS:CD2	1:A:238:ASP:H	2.18	0.61
1:B:251:ARG:HB2	1:B:291:LEU:HD21	1.82	0.60
1:C:236:HIS:CD2	1:C:238:ASP:H	2.20	0.60
1:B:302:GLU:HA	1:B:333:LEU:HD13	1.84	0.59
1:C:322:ASP:HA	1:C:325:LYS:HD3	1.84	0.59
1:C:389:TYR:HB3	1:C:455:LEU:HD12	1.83	0.59
1:A:248:LEU:HD21	2:D:1001:UNK:O	2.03	0.57
1:B:236:HIS:CD2	1:B:238:ASP:H	2.21	0.57
1:C:222:LYS:HD3	1:C:245:ILE:HB	1.87	0.56
1:B:202:HIS:HB3	1:B:225:LEU:HD11	1.88	0.56
1:B:456:GLY:HA2	1:B:471:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:GLN:HB2	1:B:339:LYS:HG3	1.90	0.54
1:A:222:LYS:NZ	1:A:246:LEU:HA	2.23	0.53
1:C:202:HIS:HB3	1:C:225:LEU:HD11	1.89	0.53
1:B:389:TYR:HD1	1:B:451:THR:HG23	1.73	0.53
1:B:320:HIS:O	1:B:323:VAL:HB	2.08	0.52
1:B:203:ASN:HA	1:B:206:ILE:HD12	1.90	0.52
1:A:202:HIS:HB3	1:A:225:LEU:HD11	1.91	0.52
1:B:330:LEU:HD12	1:B:333:LEU:HD12	1.91	0.52
1:C:203:ASN:HA	1:C:206:ILE:HD12	1.91	0.52
1:A:222:LYS:HE2	1:A:245:ILE:HG22	1.91	0.52
1:C:418:ARG:HH11	1:C:470:THR:HG23	1.75	0.51
1:B:277:ASP:HA	1:B:311:ILE:HG12	1.92	0.51
1:A:389:TYR:HD1	1:A:451:THR:HG23	1.76	0.51
1:C:389:TYR:CB	1:C:455:LEU:HD12	2.41	0.51
1:A:401:PHE:HB3	1:A:408:ASN:HD21	1.76	0.50
1:A:203:ASN:HA	1:A:206:ILE:HD12	1.95	0.49
1:C:215:GLU:HB3	1:C:253:GLN:HE21	1.77	0.49
1:B:215:GLU:HB3	1:B:253:GLN:HE21	1.78	0.48
1:B:222:LYS:HZ2	1:B:245:ILE:C	2.17	0.48
1:B:460:ARG:HG3	1:B:468:ALA:HB1	1.96	0.48
1:A:453:ARG:HH22	1:A:476:SER:HB3	1.77	0.48
1:C:277:ASP:HA	1:C:311:ILE:HG12	1.96	0.48
1:B:453:ARG:HH22	1:B:476:SER:HB3	1.78	0.47
1:C:389:TYR:HD1	1:C:451:THR:HG23	1.79	0.47
1:C:401:PHE:HB3	1:C:408:ASN:HD21	1.78	0.47
1:C:270:ARG:HB3	1:C:281:VAL:HG22	1.95	0.47
1:C:453:ARG:HG2	1:C:475:ALA:HB1	1.96	0.47
1:B:401:PHE:HB3	1:B:408:ASN:HD21	1.79	0.47
1:C:246:LEU:O	1:C:250:TYR:HD2	1.98	0.47
1:C:312:ARG:HD3	1:C:326:GLN:NE2	2.28	0.47
1:A:215:GLU:HB3	1:A:253:GLN:HE21	1.79	0.46
1:B:347:TYR:CE2	1:B:371:ASN:HB3	2.50	0.46
1:A:206:ILE:HG12	1:A:222:LYS:HG2	1.98	0.46
1:B:219:PRO:HG3	1:B:249:VAL:HG11	1.98	0.46
1:A:206:ILE:HD11	1:A:225:LEU:HG	1.98	0.45
1:A:328:SER:O	1:A:332:LEU:HD12	2.16	0.45
1:C:206:ILE:HD11	1:C:225:LEU:HG	1.98	0.45
1:C:205:VAL:HA	1:C:208:TYR:HB3	1.98	0.45
1:C:305:CYS:HB3	1:C:330:LEU:HD13	1.98	0.45
1:A:277:ASP:HA	1:A:311:ILE:HG12	1.98	0.45
1:A:270:ARG:HG2	1:A:274:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:THR:HG22	1:B:394:THR:HG21	1.98	0.45
1:C:305:CYS:HB3	1:C:330:LEU:CD1	2.47	0.44
1:B:222:LYS:HD3	1:B:245:ILE:HB	1.98	0.44
1:B:326:GLN:O	1:B:330:LEU:HB3	2.17	0.44
1:A:222:LYS:HZ3	1:A:246:LEU:HA	1.81	0.44
1:B:323:VAL:O	1:B:327:LEU:HD12	2.17	0.44
1:A:205:VAL:HA	1:A:208:TYR:HB3	2.00	0.44
1:A:237:PRO:HD3	1:A:273:THR:HG21	1.99	0.44
1:B:299:LYS:H	1:B:299:LYS:HE3	1.83	0.43
1:B:222:LYS:HZ3	1:B:249:VAL:HG21	1.83	0.43
1:B:270:ARG:HG2	1:B:274:LEU:HD12	2.00	0.43
1:A:251:ARG:HD2	1:A:294:LYS:NZ	2.33	0.43
1:B:320:HIS:ND1	1:B:322:ASP:HB2	2.33	0.43
1:C:299:LYS:H	1:C:299:LYS:HE3	1.84	0.43
1:C:251:ARG:HD2	1:C:294:LYS:NZ	2.34	0.43
1:B:334:CYS:HB2	1:B:343:VAL:HG22	1.95	0.43
1:A:455:LEU:HG	1:A:459:TYR:CE2	2.53	0.43
1:B:237:PRO:HD3	1:B:273:THR:HG21	2.01	0.42
1:B:205:VAL:HA	1:B:208:TYR:HB3	1.99	0.42
1:B:236:HIS:ND1	1:B:237:PRO:HD2	2.34	0.42
1:C:201:LEU:O	1:C:205:VAL:HG23	2.20	0.42
1:A:394:THR:HG21	1:B:356:THR:HG22	2.02	0.42
1:C:270:ARG:HG2	1:C:274:LEU:HD12	2.01	0.42
1:B:202:HIS:HB3	1:B:225:LEU:CD2	2.47	0.41
1:A:356:THR:HG21	1:B:412:TRP:HZ2	1.85	0.41
1:C:237:PRO:HD3	1:C:273:THR:HG21	2.02	0.41
1:A:322:ASP:HA	1:A:325:LYS:HD3	2.01	0.41
1:A:374:SER:HA	1:A:377:LEU:HD12	2.03	0.41
1:C:236:HIS:HD2	1:C:238:ASP:HB2	1.86	0.41
1:C:236:HIS:ND1	1:C:237:PRO:HD2	2.36	0.41
1:B:251:ARG:HH21	2:E:1002:UNK:HA	1.84	0.41
1:B:278:HIS:HB3	1:B:281:VAL:HG23	2.02	0.41
1:C:347:TYR:CE2	1:C:371:ASN:HB3	2.56	0.41
1:A:236:HIS:ND1	1:A:237:PRO:HD2	2.36	0.40
1:A:201:LEU:O	1:A:205:VAL:HG23	2.21	0.40
1:A:299:LYS:HE3	1:A:299:LYS:H	1.85	0.40
1:B:312:ARG:NH2	1:B:325:LYS:HD2	2.37	0.40
1:B:374:SER:HA	1:B:377:LEU:HD12	2.02	0.40
1:B:251:ARG:HD2	1:B:294:LYS:NZ	2.37	0.40
1:B:201:LEU:O	1:B:205:VAL:HG23	2.21	0.40
1:B:370:ASN:O	1:B:373:ALA:HB3	2.20	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	263/324 (81%)	243 (92%)	17 (6%)	3 (1%)	17	64
1	B	263/324 (81%)	237 (90%)	22 (8%)	4 (2%)	13	58
1	C	263/324 (81%)	240 (91%)	19 (7%)	4 (2%)	13	58
All	All	789/972 (81%)	720 (91%)	58 (7%)	11 (1%)	14	59

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	HIS
1	B	236	HIS
1	B	340	ALA
1	C	236	HIS
1	A	403	SER
1	C	403	SER
1	B	403	SER
1	A	197	LEU
1	B	197	LEU
1	C	197	LEU
1	C	472	GLU

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	223/268 (83%)	202 (91%)	21 (9%)	11	45
1	B	223/268 (83%)	192 (86%)	31 (14%)	4	29
1	C	223/268 (83%)	194 (87%)	29 (13%)	5	31
All	All	669/804 (83%)	588 (88%)	81 (12%)	6	33

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	197	LEU
1	A	201	LEU
1	A	203	ASN
1	A	204	LEU
1	A	211	GLN
1	A	213	ARG
1	A	214	TYR
1	A	221	CYS
1	A	242	MET
1	A	244	ASN
1	A	251	ARG
1	A	264	ASN
1	A	299	LYS
1	A	352	GLU
1	A	378	LYS
1	A	398	GLU
1	A	407	GLU
1	A	453	ARG
1	A	461	ARG
1	A	465	LEU
1	A	477	ARG
1	B	197	LEU
1	B	201	LEU
1	B	203	ASN
1	B	204	LEU
1	B	211	GLN
1	B	213	ARG
1	B	214	TYR
1	B	221	CYS
1	B	225	LEU
1	B	242	MET
1	B	244	ASN
1	B	251	ARG
1	B	264	ASN

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Mol	Chain	Res	Type
1	B	299	LYS
1	B	312	ARG
1	B	322	ASP
1	B	325	LYS
1	B	327	LEU
1	B	352	GLU
1	B	375	CYS
1	B	378	LYS
1	B	395	ARG
1	B	398	GLU
1	B	407	GLU
1	B	452	LEU
1	B	453	ARG
1	B	461	ARG
1	B	465	LEU
1	B	466	GLU
1	B	474	CYS
1	B	477	ARG
1	C	197	LEU
1	C	201	LEU
1	C	203	ASN
1	C	204	LEU
1	C	211	GLN
1	C	213	ARG
1	C	214	TYR
1	C	221	CYS
1	C	222	LYS
1	C	225	LEU
1	C	242	MET
1	C	244	ASN
1	C	251	ARG
1	C	264	ASN
1	C	299	LYS
1	C	322	ASP
1	C	326	GLN
1	C	352	GLU
1	C	375	CYS
1	C	378	LYS
1	C	398	GLU
1	C	407	GLU
1	C	453	ARG
1	C	465	LEU

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Mol	Chain	Res	Type
1	C	469	HIS
1	C	470	THR
1	C	471	LEU
1	C	476	SER
1	C	477	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	HIS
1	A	253	GLN
1	B	236	HIS
1	B	253	GLN
1	B	371	ASN
1	C	236	HIS
1	C	253	GLN
1	C	326	GLN
1	C	335	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)

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(Å²)	Q<0.9
1	A	267/324 (82%)	-0.07	4 (1%)	76	66	154, 257, 297, 300	0
1	B	267/324 (82%)	-0.09	2 (0%)	89	84	156, 264, 299, 300	0
1	C	267/324 (82%)	0.06	9 (3%)	49	37	243, 287, 300, 300	0
2	D	0/5	-	-			-	-
2	E	0/5	-	-			-	-
2	F	0/5	-	-			-	-
All	All	801/987 (81%)	-0.03	15 (1%)	70	59	154, 273, 300, 300	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	295	ARG	4.3
1	A	409	LYS	3.3
1	A	407	GLU	3.2
1	C	330	LEU	3.1
1	C	281	VAL	3.1
1	C	302	GLU	2.9
1	C	297	LYS	2.8
1	C	339	LYS	2.8
1	A	404	VAL	2.7
1	C	298	TYR	2.6
1	C	343	VAL	2.5
1	A	443	VAL	2.4
1	C	346	TYR	2.3
1	B	404	VAL	2.3
1	B	338	GLY	2.2

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.