



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:04 PM UTC

PDB ID : 5OJF / pdb_00005ojf
Title : Crystal Structure of KLC2-TPR domain (fragment [A1-B6])
Authors : Nguyen, T.Q.; Chenon, M.; Vilela, F.; Velours, C.; Andreani, J.; Fernandez-Varela, P.; Llinas, P.; Menetrey, J.
Deposited on : 2017-07-21
Resolution : 3.40 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

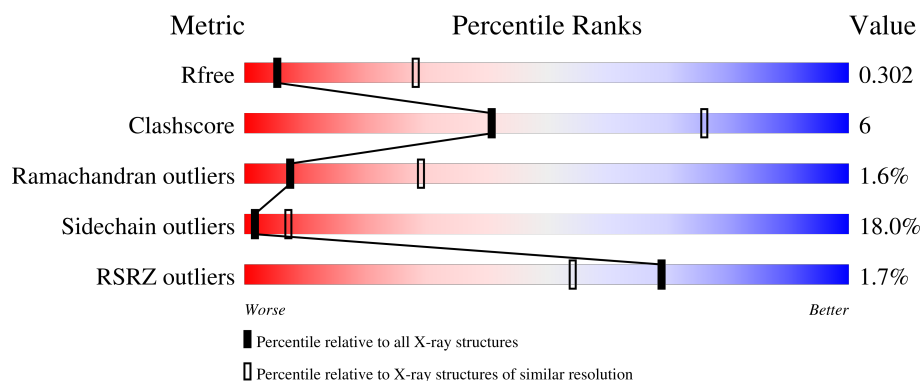
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	314	% 57% 23% • • 17%
1	B	314	2% 55% 24% • 17%
1	C	314	% 55% 25% • 17%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6255 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	262	Total	C	N	O	S	0	0	0
			2085	1305	381	392	7			
1	B	262	Total	C	N	O	S	0	0	0
			2085	1305	381	392	7			
1	C	262	Total	C	N	O	S	0	0	0
			2085	1305	381	392	7			

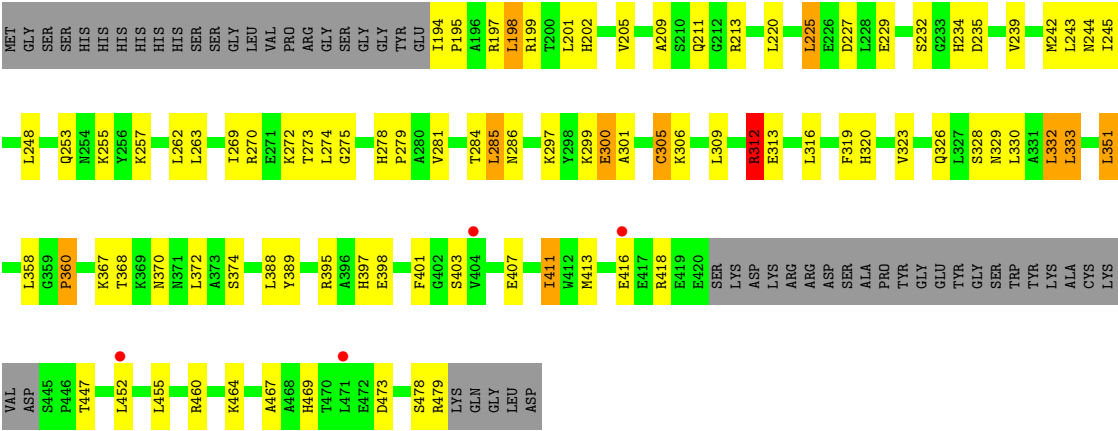
There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	MET	-	initiating methionine	UNP Q91YS4
A	172	GLY	-	expression tag	UNP Q91YS4
A	173	SER	-	expression tag	UNP Q91YS4
A	174	SER	-	expression tag	UNP Q91YS4
A	175	HIS	-	expression tag	UNP Q91YS4
A	176	HIS	-	expression tag	UNP Q91YS4
A	177	HIS	-	expression tag	UNP Q91YS4
A	178	HIS	-	expression tag	UNP Q91YS4
A	179	HIS	-	expression tag	UNP Q91YS4
A	180	HIS	-	expression tag	UNP Q91YS4
A	181	SER	-	expression tag	UNP Q91YS4
A	182	SER	-	expression tag	UNP Q91YS4
A	183	GLY	-	expression tag	UNP Q91YS4
A	184	LEU	-	expression tag	UNP Q91YS4
A	185	VAL	-	expression tag	UNP Q91YS4
A	186	PRO	-	expression tag	UNP Q91YS4
A	187	ARG	-	expression tag	UNP Q91YS4
A	188	GLY	-	expression tag	UNP Q91YS4
A	189	SER	-	expression tag	UNP Q91YS4
B	171	MET	-	initiating methionine	UNP Q91YS4
B	172	GLY	-	expression tag	UNP Q91YS4
B	173	SER	-	expression tag	UNP Q91YS4
B	174	SER	-	expression tag	UNP Q91YS4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	175	HIS	-	expression tag	UNP Q91YS4
B	176	HIS	-	expression tag	UNP Q91YS4
B	177	HIS	-	expression tag	UNP Q91YS4
B	178	HIS	-	expression tag	UNP Q91YS4
B	179	HIS	-	expression tag	UNP Q91YS4
B	180	HIS	-	expression tag	UNP Q91YS4
B	181	SER	-	expression tag	UNP Q91YS4
B	182	SER	-	expression tag	UNP Q91YS4
B	183	GLY	-	expression tag	UNP Q91YS4
B	184	LEU	-	expression tag	UNP Q91YS4
B	185	VAL	-	expression tag	UNP Q91YS4
B	186	PRO	-	expression tag	UNP Q91YS4
B	187	ARG	-	expression tag	UNP Q91YS4
B	188	GLY	-	expression tag	UNP Q91YS4
B	189	SER	-	expression tag	UNP Q91YS4
C	171	MET	-	initiating methionine	UNP Q91YS4
C	172	GLY	-	expression tag	UNP Q91YS4
C	173	SER	-	expression tag	UNP Q91YS4
C	174	SER	-	expression tag	UNP Q91YS4
C	175	HIS	-	expression tag	UNP Q91YS4
C	176	HIS	-	expression tag	UNP Q91YS4
C	177	HIS	-	expression tag	UNP Q91YS4
C	178	HIS	-	expression tag	UNP Q91YS4
C	179	HIS	-	expression tag	UNP Q91YS4
C	180	HIS	-	expression tag	UNP Q91YS4
C	181	SER	-	expression tag	UNP Q91YS4
C	182	SER	-	expression tag	UNP Q91YS4
C	183	GLY	-	expression tag	UNP Q91YS4
C	184	LEU	-	expression tag	UNP Q91YS4
C	185	VAL	-	expression tag	UNP Q91YS4
C	186	PRO	-	expression tag	UNP Q91YS4
C	187	ARG	-	expression tag	UNP Q91YS4
C	188	GLY	-	expression tag	UNP Q91YS4
C	189	SER	-	expression tag	UNP Q91YS4



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	97.62Å 116.47Å 108.11Å 90.00° 99.51° 90.00°	Depositor
Resolution (Å)	20.00 – 3.40 20.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-3.40) 99.4 (20.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.232 , 0.264 0.261 , 0.302	Depositor DCC
R_{free} test set	830 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	104.9	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 140.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6255	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.36 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2291e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.93	0/2120	1.60	30/2861 (1.0%)
1	B	0.91	0/2120	1.61	35/2861 (1.2%)
1	C	0.89	0/2120	1.59	26/2861 (0.9%)
All	All	0.91	0/6360	1.60	91/8583 (1.1%)

There are no bond length outliers.

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	473	ASP	CA-CB-CG	7.61	120.20	112.60
1	B	473	ASP	CA-CB-CG	7.58	120.17	112.60
1	A	473	ASP	CA-CB-CG	7.31	119.91	112.60
1	A	253	GLN	CA-C-N	6.54	134.03	121.54
1	A	253	GLN	C-N-CA	6.54	134.03	121.54
1	C	253	GLN	CA-C-N	6.50	133.95	121.54
1	C	253	GLN	C-N-CA	6.50	133.95	121.54
1	B	253	GLN	CA-C-N	6.47	133.89	121.54
1	B	253	GLN	C-N-CA	6.47	133.89	121.54
1	A	332	LEU	CA-C-N	6.15	129.02	120.29
1	A	332	LEU	C-N-CA	6.15	129.02	120.29
1	C	285	LEU	N-CA-C	-6.07	105.71	113.23
1	C	255	LYS	CA-C-N	6.04	128.65	120.38
1	C	255	LYS	C-N-CA	6.04	128.65	120.38
1	B	213	ARG	CA-C-N	6.03	128.36	120.28
1	B	213	ARG	C-N-CA	6.03	128.36	120.28
1	A	265	ASP	CA-CB-CG	6.02	118.62	112.60
1	C	213	ARG	CA-C-N	6.01	128.33	120.28
1	C	213	ARG	C-N-CA	6.01	128.33	120.28
1	B	332	LEU	CA-C-N	5.98	128.78	120.29
1	B	332	LEU	C-N-CA	5.98	128.78	120.29
1	B	411	ILE	N-CA-CB	5.90	117.06	110.51
1	A	213	ARG	CA-C-N	5.83	128.09	120.28
1	A	213	ARG	C-N-CA	5.83	128.09	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	ARG	CA-C-N	5.81	128.07	120.28
1	A	312	ARG	C-N-CA	5.81	128.07	120.28
1	B	265	ASP	CA-CB-CG	5.79	118.39	112.60
1	B	312	ARG	CA-C-N	5.79	128.03	120.28
1	B	312	ARG	C-N-CA	5.79	128.03	120.28
1	C	411	ILE	N-CA-CB	5.75	116.90	110.51
1	B	285	LEU	N-CA-C	-5.74	106.12	113.23
1	A	411	ILE	N-CA-CB	5.73	116.87	110.51
1	C	332	LEU	CA-C-N	5.72	128.41	120.29
1	C	332	LEU	C-N-CA	5.72	128.41	120.29
1	B	198	LEU	CA-C-N	5.68	128.47	120.28
1	B	198	LEU	C-N-CA	5.68	128.47	120.28
1	A	307	ARG	CA-C-N	5.67	128.93	120.31
1	A	307	ARG	C-N-CA	5.67	128.93	120.31
1	B	255	LYS	CA-C-N	5.65	128.12	120.38
1	B	255	LYS	C-N-CA	5.65	128.12	120.38
1	C	329	ASN	CA-CB-CG	5.65	118.25	112.60
1	C	312	ARG	CA-C-N	5.62	127.81	120.28
1	C	312	ARG	C-N-CA	5.62	127.81	120.28
1	A	255	LYS	CA-C-N	5.59	128.04	120.38
1	A	255	LYS	C-N-CA	5.59	128.04	120.38
1	B	329	ASN	CA-CB-CG	5.55	118.15	112.60
1	C	198	LEU	CA-C-N	5.55	128.28	120.28
1	C	198	LEU	C-N-CA	5.55	128.28	120.28
1	A	198	LEU	CA-C-N	5.55	128.28	120.28
1	A	198	LEU	C-N-CA	5.55	128.28	120.28
1	B	205	VAL	CA-C-N	5.49	128.28	120.53
1	B	205	VAL	C-N-CA	5.49	128.28	120.53
1	C	205	VAL	CA-C-N	5.49	128.27	120.53
1	C	205	VAL	C-N-CA	5.49	128.27	120.53
1	A	285	LEU	N-CA-C	-5.36	106.24	112.89
1	A	202	HIS	CA-C-N	5.35	128.20	120.38
1	A	202	HIS	C-N-CA	5.35	128.20	120.38
1	A	205	VAL	CA-C-N	5.35	128.08	120.53
1	A	205	VAL	C-N-CA	5.35	128.08	120.53
1	C	202	HIS	CA-C-N	5.34	128.18	120.38
1	C	202	HIS	C-N-CA	5.34	128.18	120.38
1	A	239	VAL	N-CA-C	-5.33	105.19	111.00
1	B	239	VAL	N-CA-C	-5.26	105.27	111.00
1	B	299	LYS	CA-C-N	5.26	130.91	121.66
1	B	299	LYS	C-N-CA	5.26	130.91	121.66
1	C	239	VAL	N-CA-C	-5.23	105.30	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	HIS	CA-C-N	5.20	127.98	120.38
1	B	202	HIS	C-N-CA	5.20	127.98	120.38
1	A	369	LYS	CA-C-N	5.17	127.46	120.38
1	A	369	LYS	C-N-CA	5.17	127.46	120.38
1	A	196	ALA	CA-C-N	5.16	127.47	120.65
1	A	196	ALA	C-N-CA	5.16	127.47	120.65
1	B	331	ALA	CA-C-N	5.15	127.18	120.28
1	B	331	ALA	C-N-CA	5.15	127.18	120.28
1	B	209	ALA	N-CA-C	-5.11	106.13	112.93
1	A	473	ASP	N-CA-C	-5.08	105.20	111.40
1	C	299	LYS	CA-C-N	5.08	130.59	121.66
1	C	299	LYS	C-N-CA	5.08	130.59	121.66
1	B	398	GLU	CA-C-N	5.07	127.34	120.44
1	B	398	GLU	C-N-CA	5.07	127.34	120.44
1	C	323	VAL	N-CA-C	-5.04	105.50	111.00
1	A	299	LYS	CA-C-N	5.03	130.52	121.66
1	A	299	LYS	C-N-CA	5.03	130.52	121.66
1	B	196	ALA	CA-C-N	5.03	127.29	120.65
1	B	196	ALA	C-N-CA	5.03	127.29	120.65
1	C	469	HIS	CA-C-N	5.02	127.32	120.54
1	C	469	HIS	C-N-CA	5.02	127.32	120.54
1	B	348	ARG	CA-C-N	5.02	127.42	120.29
1	B	348	ARG	C-N-CA	5.02	127.42	120.29
1	B	469	HIS	CA-C-N	5.01	127.30	120.54
1	B	469	HIS	C-N-CA	5.01	127.30	120.54

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	2085	0	2102	26	0
1	B	2085	0	2102	27	0
1	C	2085	0	2102	30	0
All	All	6255	0	6306	81	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 6.

All (81) 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:225:LEU:HD12	1:B:242:MET:HB3	1.61	0.81
1:A:225:LEU:HD12	1:A:242:MET:HB3	1.64	0.80
1:C:225:LEU:HD12	1:C:242:MET:HB3	1.62	0.78
1:A:309:LEU:HD12	1:A:326:GLN:HG3	1.70	0.73
1:B:309:LEU:HD12	1:B:326:GLN:HG3	1.85	0.58
1:A:270:ARG:HB3	1:A:281:VAL:HG22	1.86	0.57
1:B:270:ARG:HB3	1:B:281:VAL:HG22	1.86	0.56
1:A:312:ARG:HG3	1:A:316:LEU:HD12	1.88	0.56
1:C:270:ARG:HB3	1:C:281:VAL:HG22	1.87	0.54
1:B:305:CYS:HB3	1:B:330:LEU:HD13	1.88	0.54
1:C:312:ARG:HG3	1:C:316:LEU:HD12	1.89	0.53
1:C:305:CYS:HB3	1:C:330:LEU:HD13	1.90	0.53
1:B:198:LEU:HB3	1:B:242:MET:HE3	1.91	0.53
1:C:198:LEU:HB3	1:C:242:MET:HE3	1.93	0.50
1:A:198:LEU:HB3	1:A:242:MET:HE3	1.94	0.50
1:B:225:LEU:HD11	1:B:243:LEU:HG	1.95	0.48
1:B:397:HIS:O	1:B:401:PHE:HB2	2.13	0.48
1:A:305:CYS:HB3	1:A:330:LEU:HD13	1.95	0.48
1:C:397:HIS:O	1:C:401:PHE:HB2	2.13	0.48
1:A:225:LEU:HD11	1:A:243:LEU:HG	1.96	0.48
1:C:225:LEU:HD11	1:C:243:LEU:HG	1.96	0.48
1:B:209:ALA:C	1:B:211:GLN:H	2.22	0.47
1:B:198:LEU:HD13	1:B:242:MET:HG2	1.96	0.47
1:A:209:ALA:C	1:A:211:GLN:H	2.22	0.47
1:A:397:HIS:O	1:A:401:PHE:HB2	2.14	0.47
1:B:310:GLU:O	1:B:314:LYS:HG2	2.16	0.46
1:C:464:LYS:HB3	1:C:467:ALA:HB3	1.97	0.46
1:A:413:MET:HE2	1:C:319:PHE:HB3	1.97	0.46
1:C:395:ARG:HH11	1:C:398:GLU:HB3	1.80	0.46
1:A:198:LEU:HD13	1:A:242:MET:HG2	1.98	0.46
1:A:275:GLY:O	1:A:281:VAL:HG21	2.16	0.46
1:B:308:ALA:HB3	1:B:326:GLN:NE2	2.30	0.46
1:B:464:LYS:HB3	1:B:467:ALA:HB3	1.97	0.46
1:A:309:LEU:HD13	1:A:330:LEU:HD22	1.98	0.46
1:C:209:ALA:C	1:C:211:GLN:H	2.23	0.46
1:B:351:LEU:HD22	1:B:368:THR:HG22	1.97	0.46
1:A:301:ALA:HB3	1:A:333:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:PRO:HD2	1:C:198:LEU:HB2	1.98	0.45
1:C:275:GLY:O	1:C:281:VAL:HG21	2.16	0.45
1:A:464:LYS:HB3	1:A:467:ALA:HB3	1.99	0.45
1:A:395:ARG:HH11	1:A:398:GLU:HB3	1.82	0.45
1:C:351:LEU:HD22	1:C:368:THR:HG22	1.97	0.45
1:B:195:PRO:HD2	1:B:198:LEU:HB2	1.98	0.45
1:B:395:ARG:HH11	1:B:398:GLU:HB3	1.81	0.45
1:C:198:LEU:HD13	1:C:242:MET:HG2	1.99	0.45
1:B:275:GLY:O	1:B:281:VAL:HG21	2.17	0.45
1:A:319:PHE:HB3	1:C:413:MET:HE2	2.00	0.44
1:B:301:ALA:HB3	1:B:333:LEU:HD21	1.99	0.44
1:A:195:PRO:HD2	1:A:198:LEU:HB2	1.99	0.44
1:C:301:ALA:HB3	1:C:333:LEU:HD21	2.00	0.44
1:C:263:LEU:HD23	1:C:263:LEU:HA	1.86	0.44
1:A:351:LEU:HD22	1:A:368:THR:HG22	1.99	0.43
1:B:297:LYS:HB3	1:B:300:GLU:HG3	2.01	0.43
1:A:316:LEU:HD22	1:A:320:HIS:CE1	2.54	0.43
1:B:316:LEU:HD22	1:B:320:HIS:CE1	2.54	0.43
1:B:389:TYR:HB3	1:B:455:LEU:HB2	2.01	0.43
1:A:331:ALA:HB2	1:A:346:TYR:HB2	2.01	0.43
1:A:389:TYR:HB3	1:A:455:LEU:HB2	2.01	0.43
1:A:225:LEU:HD12	1:A:242:MET:CB	2.44	0.43
1:A:195:PRO:O	1:A:199:ARG:HB2	2.19	0.42
1:B:195:PRO:O	1:B:199:ARG:HB2	2.19	0.42
1:B:405:ASN:HB2	1:B:408:ASN:H	1.85	0.42
1:C:297:LYS:HB3	1:C:300:GLU:HG3	2.01	0.42
1:C:309:LEU:HD12	1:C:326:GLN:HG3	2.01	0.42
1:C:360:PRO:HB2	1:C:395:ARG:HE	1.85	0.42
1:C:395:ARG:NH1	1:C:398:GLU:HB3	2.35	0.42
1:A:281:VAL:O	1:A:285:LEU:HD12	2.21	0.41
1:B:195:PRO:HG2	1:B:198:LEU:HD12	2.02	0.41
1:C:270:ARG:HG2	1:C:274:LEU:HD12	2.02	0.41
1:C:278:HIS:CD2	1:C:279:PRO:HD2	2.55	0.41
1:C:316:LEU:HD22	1:C:320:HIS:CE1	2.54	0.41
1:B:225:LEU:HD12	1:B:242:MET:CB	2.42	0.41
1:C:234:HIS:CE1	1:C:269:ILE:HD11	2.54	0.41
1:B:270:ARG:HG2	1:B:274:LEU:HD12	2.02	0.41
1:A:297:LYS:HB3	1:A:300:GLU:HG3	2.03	0.41
1:B:281:VAL:O	1:B:285:LEU:HD12	2.21	0.41
1:B:311:ILE:O	1:B:315:VAL:HG23	2.21	0.41
1:C:389:TYR:HB3	1:C:455:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:LEU:HD12	1:C:242:MET:CB	2.43	0.40
1:C:281:VAL:HA	1:C:284:THR:HG22	2.03	0.40
1:C:372:LEU:HD23	1:C:388:LEU:HD11	2.02	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	258/314 (82%)	235 (91%)	19 (7%)	4 (2%)	7	29
1	B	258/314 (82%)	235 (91%)	19 (7%)	4 (2%)	7	29
1	C	258/314 (82%)	235 (91%)	19 (7%)	4 (2%)	7	29
All	All	774/942 (82%)	705 (91%)	57 (7%)	12 (2%)	7	29

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	PRO
1	A	478	SER
1	B	360	PRO
1	B	478	SER
1	C	360	PRO
1	C	478	SER
1	A	235	ASP
1	B	235	ASP
1	C	235	ASP
1	C	272	LYS
1	A	272	LYS
1	B	272	LYS

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	219/261 (84%)	180 (82%)	39 (18%)	2	7
1	B	219/261 (84%)	179 (82%)	40 (18%)	2	7
1	C	219/261 (84%)	180 (82%)	39 (18%)	2	7
All	All	657/783 (84%)	539 (82%)	118 (18%)	2	7

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	ILE
1	A	197	ARG
1	A	199	ARG
1	A	201	LEU
1	A	220	LEU
1	A	225	LEU
1	A	227	ASP
1	A	229	GLU
1	A	232	SER
1	A	244	ASN
1	A	245	ILE
1	A	248	LEU
1	A	257	LYS
1	A	262	LEU
1	A	273	THR
1	A	285	LEU
1	A	286	ASN
1	A	300	GLU
1	A	305	CYS
1	A	309	LEU
1	A	312	ARG
1	A	313	GLU
1	A	328	SER
1	A	332	LEU
1	A	333	LEU
1	A	351	LEU

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Mol	Chain	Res	Type
1	A	358	LEU
1	A	367	LYS
1	A	370	ASN
1	A	374	SER
1	A	403	SER
1	A	407	GLU
1	A	411	ILE
1	A	416	GLU
1	A	418	ARG
1	A	447	THR
1	A	452	LEU
1	A	460	ARG
1	A	479	ARG
1	B	194	ILE
1	B	197	ARG
1	B	199	ARG
1	B	201	LEU
1	B	220	LEU
1	B	225	LEU
1	B	227	ASP
1	B	229	GLU
1	B	232	SER
1	B	244	ASN
1	B	245	ILE
1	B	248	LEU
1	B	257	LYS
1	B	262	LEU
1	B	273	THR
1	B	285	LEU
1	B	286	ASN
1	B	300	GLU
1	B	305	CYS
1	B	306	LYS
1	B	309	LEU
1	B	312	ARG
1	B	313	GLU
1	B	328	SER
1	B	332	LEU
1	B	333	LEU
1	B	351	LEU
1	B	358	LEU
1	B	367	LYS

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Mol	Chain	Res	Type
1	B	370	ASN
1	B	374	SER
1	B	403	SER
1	B	407	GLU
1	B	411	ILE
1	B	416	GLU
1	B	418	ARG
1	B	447	THR
1	B	452	LEU
1	B	460	ARG
1	B	479	ARG
1	C	194	ILE
1	C	197	ARG
1	C	199	ARG
1	C	201	LEU
1	C	220	LEU
1	C	225	LEU
1	C	227	ASP
1	C	229	GLU
1	C	232	SER
1	C	244	ASN
1	C	245	ILE
1	C	248	LEU
1	C	257	LYS
1	C	262	LEU
1	C	273	THR
1	C	285	LEU
1	C	286	ASN
1	C	300	GLU
1	C	305	CYS
1	C	306	LYS
1	C	312	ARG
1	C	313	GLU
1	C	328	SER
1	C	332	LEU
1	C	333	LEU
1	C	351	LEU
1	C	358	LEU
1	C	367	LYS
1	C	370	ASN
1	C	374	SER
1	C	403	SER

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Mol	Chain	Res	Type
1	C	407	GLU
1	C	411	ILE
1	C	416	GLU
1	C	418	ARG
1	C	447	THR
1	C	452	LEU
1	C	460	ARG
1	C	479	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	HIS
1	A	253	GLN
1	A	337	GLN
1	A	379	GLN
1	A	383	GLN
1	A	449	ASN
1	A	462	GLN
1	A	469	HIS
1	B	202	HIS
1	B	203	ASN
1	B	253	GLN
1	B	337	GLN
1	B	379	GLN
1	B	449	ASN
1	B	469	HIS
1	C	202	HIS
1	C	337	GLN
1	C	379	GLN
1	C	383	GLN
1	C	449	ASN
1	C	469	HIS

5.3.3 RNA ⓘ

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 oligosaccharides 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	262/314 (83%)	0.07	4 (1%)	72 57	74, 120, 169, 206	0
1	B	262/314 (83%)	0.04	5 (1%)	66 51	66, 121, 175, 213	0
1	C	262/314 (83%)	0.02	4 (1%)	72 57	82, 130, 178, 207	0
All	All	786/942 (83%)	0.04	13 (1%)	69 54	66, 124, 175, 213	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	404	VAL	2.9
1	A	450	THR	2.9
1	C	471	LEU	2.9
1	A	404	VAL	2.9
1	B	450	THR	2.6
1	A	448	VAL	2.5
1	C	452	LEU	2.4
1	B	404	VAL	2.3
1	B	448	VAL	2.3
1	B	479	ARG	2.1
1	B	445	SER	2.1
1	A	228	LEU	2.0
1	C	416	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 oligosaccharides 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.