Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2025 – 04:10 PM JST

PDB ID	:	8XLA / pdb_00008xla
Title	:	Mismatch Repair Complex
Authors	:	Nirwal, S.; Nair, D.T.
Deposited on	:	2023-12-25
Resolution	:	3.50 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:

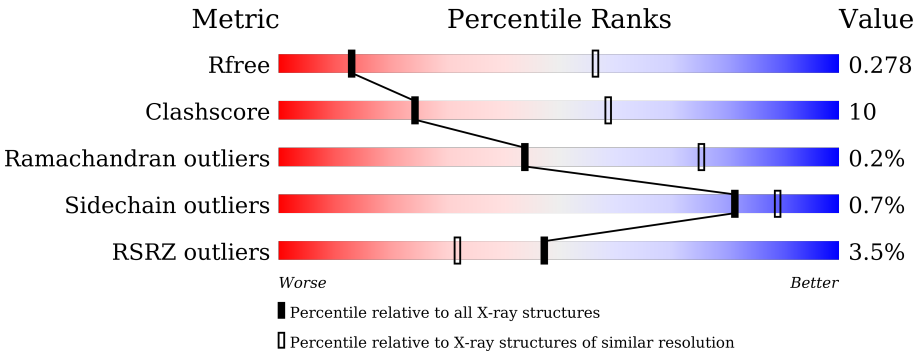
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.50 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}	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)

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 <=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	387	2% 76% 20%
1	B	387	75% 20% 5%
1	E	387	% 81% 14% 5%
1	F	387	% 79% 16% 5%
2	D	220	10% 50% 28% 20%
2	Y	220	10% 44% 40% 15%

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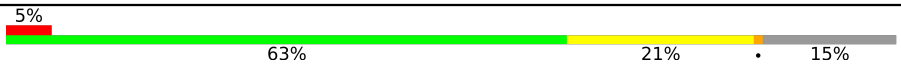
Mol	Chain	Length	Quality of chain
2	Z	220	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15581 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 Beta sliding clamp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2912	1847	505	547	13			
1	B	366	Total	C	N	O	S	0	0	0
			2865	1819	495	539	12			
1	E	367	Total	C	N	O	S	0	0	0
			2874	1824	498	539	13			
1	F	367	Total	C	N	O	S	0	0	0
			2869	1821	496	539	13			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q5FAJ1
A	-19	GLY	-	expression tag	UNP Q5FAJ1
A	-18	SER	-	expression tag	UNP Q5FAJ1
A	-17	SER	-	expression tag	UNP Q5FAJ1
A	-16	HIS	-	expression tag	UNP Q5FAJ1
A	-15	HIS	-	expression tag	UNP Q5FAJ1
A	-14	HIS	-	expression tag	UNP Q5FAJ1
A	-13	HIS	-	expression tag	UNP Q5FAJ1
A	-12	HIS	-	expression tag	UNP Q5FAJ1
A	-11	HIS	-	expression tag	UNP Q5FAJ1
A	-10	SER	-	expression tag	UNP Q5FAJ1
A	-9	SER	-	expression tag	UNP Q5FAJ1
A	-8	GLY	-	expression tag	UNP Q5FAJ1
A	-7	LEU	-	expression tag	UNP Q5FAJ1
A	-6	VAL	-	expression tag	UNP Q5FAJ1
A	-5	PRO	-	expression tag	UNP Q5FAJ1
A	-4	ARG	-	expression tag	UNP Q5FAJ1
A	-3	GLY	-	expression tag	UNP Q5FAJ1
A	-2	SER	-	expression tag	UNP Q5FAJ1
A	-1	HIS	-	expression tag	UNP Q5FAJ1
B	-19	MET	-	initiating methionine	UNP Q5FAJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q5FAJ1
B	-17	SER	-	expression tag	UNP Q5FAJ1
B	-16	SER	-	expression tag	UNP Q5FAJ1
B	-15	HIS	-	expression tag	UNP Q5FAJ1
B	-14	HIS	-	expression tag	UNP Q5FAJ1
B	-13	HIS	-	expression tag	UNP Q5FAJ1
B	-12	HIS	-	expression tag	UNP Q5FAJ1
B	-11	HIS	-	expression tag	UNP Q5FAJ1
B	-10	HIS	-	expression tag	UNP Q5FAJ1
B	-9	SER	-	expression tag	UNP Q5FAJ1
B	-8	SER	-	expression tag	UNP Q5FAJ1
B	-7	GLY	-	expression tag	UNP Q5FAJ1
B	-6	LEU	-	expression tag	UNP Q5FAJ1
B	-5	VAL	-	expression tag	UNP Q5FAJ1
B	-4	PRO	-	expression tag	UNP Q5FAJ1
B	-3	ARG	-	expression tag	UNP Q5FAJ1
B	-2	GLY	-	expression tag	UNP Q5FAJ1
B	-1	SER	-	expression tag	UNP Q5FAJ1
B	0	HIS	-	expression tag	UNP Q5FAJ1
E	-20	MET	-	initiating methionine	UNP Q5FAJ1
E	-19	GLY	-	expression tag	UNP Q5FAJ1
E	-18	SER	-	expression tag	UNP Q5FAJ1
E	-17	SER	-	expression tag	UNP Q5FAJ1
E	-16	HIS	-	expression tag	UNP Q5FAJ1
E	-15	HIS	-	expression tag	UNP Q5FAJ1
E	-14	HIS	-	expression tag	UNP Q5FAJ1
E	-13	HIS	-	expression tag	UNP Q5FAJ1
E	-12	HIS	-	expression tag	UNP Q5FAJ1
E	-11	HIS	-	expression tag	UNP Q5FAJ1
E	-10	SER	-	expression tag	UNP Q5FAJ1
E	-9	SER	-	expression tag	UNP Q5FAJ1
E	-8	GLY	-	expression tag	UNP Q5FAJ1
E	-7	LEU	-	expression tag	UNP Q5FAJ1
E	-6	VAL	-	expression tag	UNP Q5FAJ1
E	-5	PRO	-	expression tag	UNP Q5FAJ1
E	-4	ARG	-	expression tag	UNP Q5FAJ1
E	-3	GLY	-	expression tag	UNP Q5FAJ1
E	-2	SER	-	expression tag	UNP Q5FAJ1
E	-1	HIS	-	expression tag	UNP Q5FAJ1
F	-20	MET	-	initiating methionine	UNP Q5FAJ1
F	-19	GLY	-	expression tag	UNP Q5FAJ1
F	-18	SER	-	expression tag	UNP Q5FAJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-17	SER	-	expression tag	UNP Q5FAJ1
F	-16	HIS	-	expression tag	UNP Q5FAJ1
F	-15	HIS	-	expression tag	UNP Q5FAJ1
F	-14	HIS	-	expression tag	UNP Q5FAJ1
F	-13	HIS	-	expression tag	UNP Q5FAJ1
F	-12	HIS	-	expression tag	UNP Q5FAJ1
F	-11	HIS	-	expression tag	UNP Q5FAJ1
F	-10	SER	-	expression tag	UNP Q5FAJ1
F	-9	SER	-	expression tag	UNP Q5FAJ1
F	-8	GLY	-	expression tag	UNP Q5FAJ1
F	-7	LEU	-	expression tag	UNP Q5FAJ1
F	-6	VAL	-	expression tag	UNP Q5FAJ1
F	-5	PRO	-	expression tag	UNP Q5FAJ1
F	-4	ARG	-	expression tag	UNP Q5FAJ1
F	-3	GLY	-	expression tag	UNP Q5FAJ1
F	-2	SER	-	expression tag	UNP Q5FAJ1
F	-1	HIS	-	expression tag	UNP Q5FAJ1

- Molecule 2 is a protein called DNA mismatch repair protein MutL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	186	Total	C	N	O	S	0	0	0
			1409	877	256	266	10			
2	Z	187	Total	C	N	O	S	0	0	0
			1352	839	253	252	8			
2	D	176	Total	C	N	O	S	0	0	0
			1300	812	233	246	9			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	439	THR	-	expression tag	UNP Q5F8M6
Y	440	MET	-	expression tag	UNP Q5F8M6
Y	441	GLY	-	expression tag	UNP Q5F8M6
Y	442	SER	-	expression tag	UNP Q5F8M6
Y	443	SER	-	expression tag	UNP Q5F8M6
Y	444	HIS	-	expression tag	UNP Q5F8M6
Y	445	HIS	-	expression tag	UNP Q5F8M6
Y	446	HIS	-	expression tag	UNP Q5F8M6
Y	447	HIS	-	expression tag	UNP Q5F8M6
Y	448	HIS	-	expression tag	UNP Q5F8M6
Y	449	HIS	-	expression tag	UNP Q5F8M6

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	450	SER	-	expression tag	UNP Q5F8M6
Y	451	SER	-	expression tag	UNP Q5F8M6
Y	452	GLY	-	expression tag	UNP Q5F8M6
Y	453	LEU	-	expression tag	UNP Q5F8M6
Y	454	VAL	-	expression tag	UNP Q5F8M6
Y	455	PRO	-	expression tag	UNP Q5F8M6
Y	456	ARG	-	expression tag	UNP Q5F8M6
Y	457	GLY	-	expression tag	UNP Q5F8M6
Y	458	SER	-	expression tag	UNP Q5F8M6
Y	459	HIS	-	expression tag	UNP Q5F8M6
Z	439	THR	-	expression tag	UNP Q5F8M6
Z	440	MET	-	expression tag	UNP Q5F8M6
Z	441	GLY	-	expression tag	UNP Q5F8M6
Z	442	SER	-	expression tag	UNP Q5F8M6
Z	443	SER	-	expression tag	UNP Q5F8M6
Z	444	HIS	-	expression tag	UNP Q5F8M6
Z	445	HIS	-	expression tag	UNP Q5F8M6
Z	446	HIS	-	expression tag	UNP Q5F8M6
Z	447	HIS	-	expression tag	UNP Q5F8M6
Z	448	HIS	-	expression tag	UNP Q5F8M6
Z	449	HIS	-	expression tag	UNP Q5F8M6
Z	450	SER	-	expression tag	UNP Q5F8M6
Z	451	SER	-	expression tag	UNP Q5F8M6
Z	452	GLY	-	expression tag	UNP Q5F8M6
Z	453	LEU	-	expression tag	UNP Q5F8M6
Z	454	VAL	-	expression tag	UNP Q5F8M6
Z	455	PRO	-	expression tag	UNP Q5F8M6
Z	456	ARG	-	expression tag	UNP Q5F8M6
Z	457	GLY	-	expression tag	UNP Q5F8M6
Z	458	SER	-	expression tag	UNP Q5F8M6
Z	459	HIS	-	expression tag	UNP Q5F8M6
D	439	THR	-	expression tag	UNP Q5F8M6
D	440	MET	-	expression tag	UNP Q5F8M6
D	441	GLY	-	expression tag	UNP Q5F8M6
D	442	SER	-	expression tag	UNP Q5F8M6
D	443	SER	-	expression tag	UNP Q5F8M6
D	444	HIS	-	expression tag	UNP Q5F8M6
D	445	HIS	-	expression tag	UNP Q5F8M6
D	446	HIS	-	expression tag	UNP Q5F8M6
D	447	HIS	-	expression tag	UNP Q5F8M6
D	448	HIS	-	expression tag	UNP Q5F8M6
D	449	HIS	-	expression tag	UNP Q5F8M6

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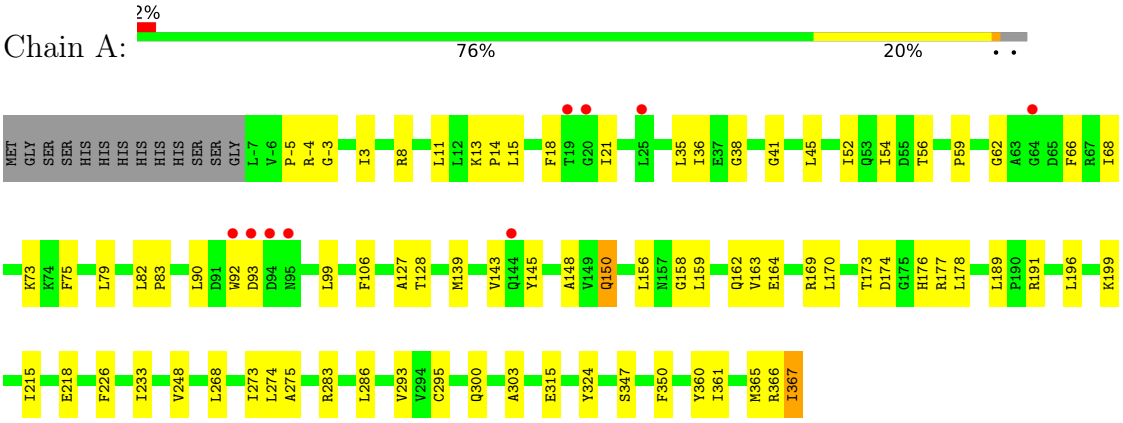
Chain	Residue	Modelled	Actual	Comment	Reference
D	450	SER	-	expression tag	UNP Q5F8M6
D	451	SER	-	expression tag	UNP Q5F8M6
D	452	GLY	-	expression tag	UNP Q5F8M6
D	453	LEU	-	expression tag	UNP Q5F8M6
D	454	VAL	-	expression tag	UNP Q5F8M6
D	455	PRO	-	expression tag	UNP Q5F8M6
D	456	ARG	-	expression tag	UNP Q5F8M6
D	457	GLY	-	expression tag	UNP Q5F8M6
D	458	SER	-	expression tag	UNP Q5F8M6
D	459	HIS	-	expression tag	UNP Q5F8M6

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.

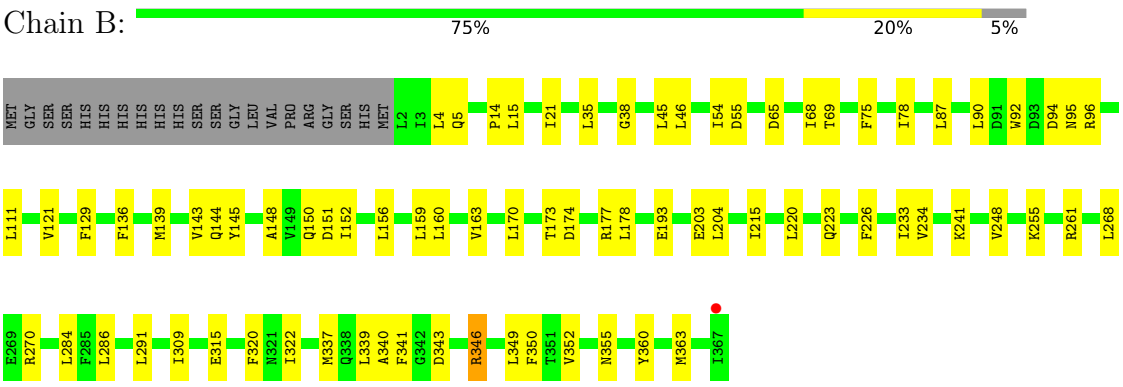
• Molecule 1: Beta sliding clamp

Chain A:



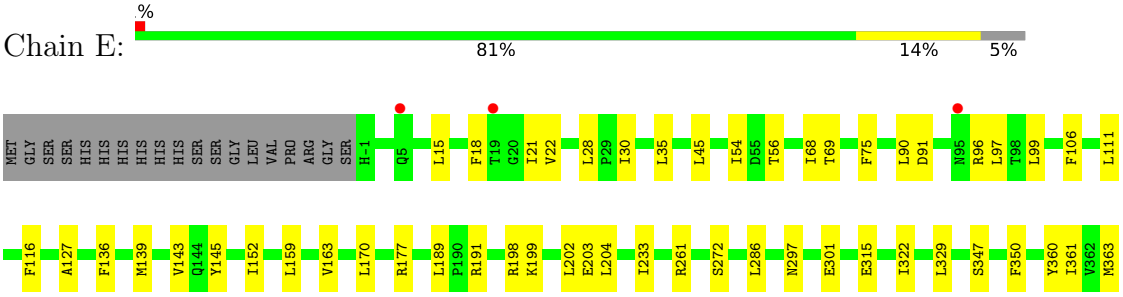
• Molecule 1: Beta sliding clamp

Chain B:

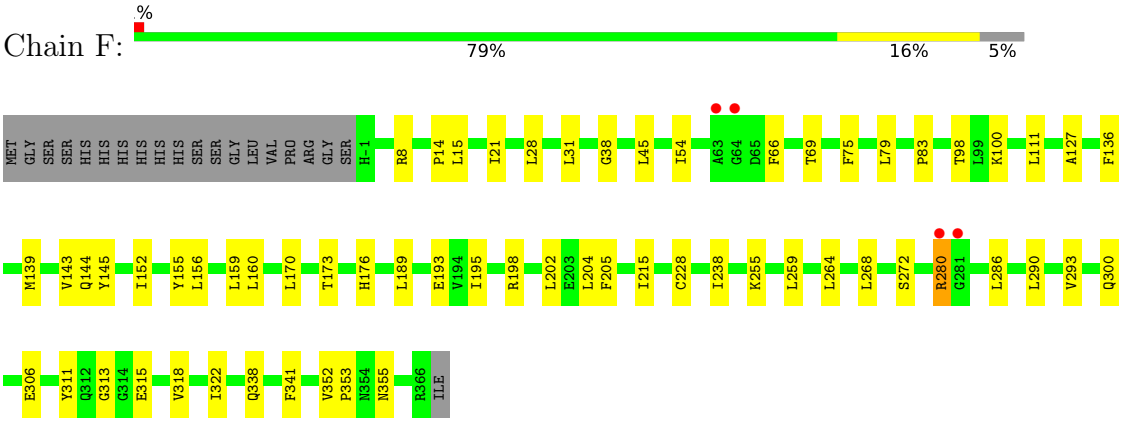


• Molecule 1: Beta sliding clamp

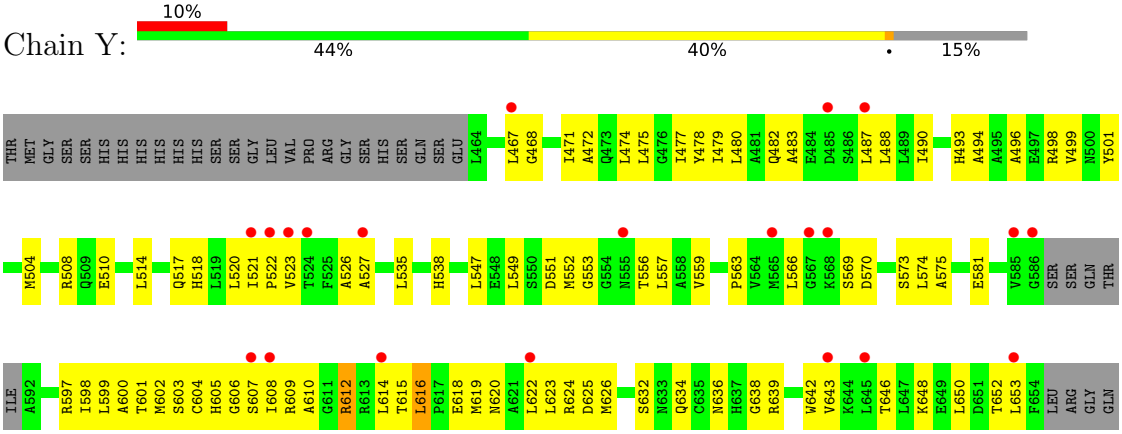
Chain E:



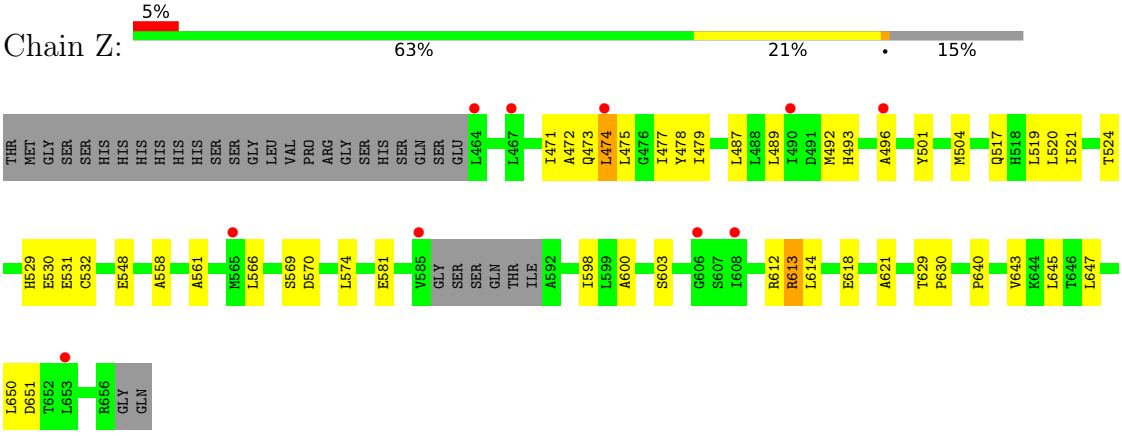
• Molecule 1: Beta sliding clamp



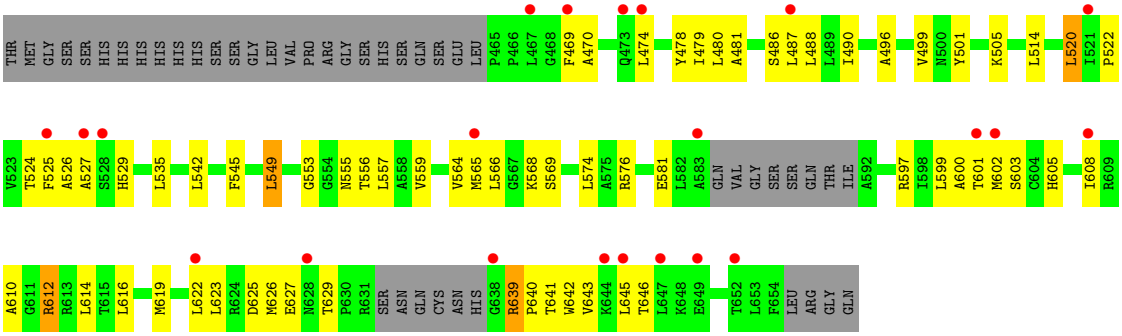
• Molecule 2: DNA mismatch repair protein MutL



• Molecule 2: DNA mismatch repair protein MutL



• Molecule 2: DNA mismatch repair protein MutL


THR MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS SER GLN SER GLU LEU P465 P466 L467 G468 F469 A470 Q473 L474 Y478 I479 L480 A481 S486 L487 L488 L489 I490 A496 V499 N500 Y501 K505 L514 L520 I521 P522
V523 T524 F525 A526 A527 S528 H529 L535 L542 F545 L549 G553 G554 N555 T556 L557 A558 V559 V564 M565 L566 G567 K568 S569 L574 A575 R576 E581 L582 A583 GLN VAL GLY SER SER GLN THR ILE A592 R597 I598 L599 A600 T601 M602 S603 C604 H605 I608 R609
A610 G611 R612 R613 L614 T615 L616 M619 L622 L623 R624 D625 M626 E627 M628 T629 P630 R631 SER ASN GLN CYS ASN HIS G638 R639 P640 T641 W642 V643 K644 L645 T646 L647 K648 E649 T652 L653 F654 LEU ARG GLY GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	160.75Å 212.04Å 255.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.70 – 3.50 64.70 – 3.50	Depositor EDS
% Data completeness (in resolution range)	95.6 (64.70-3.50) 97.7 (64.70-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.267 , 0.280 0.266 , 0.278	Depositor DCC
R_{free} test set	2786 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	114.7	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 93.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	15581	wwPDB-VP
Average B, all atoms (Å^2)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.43	3/2958 (0.1%)	0.59	2/4002 (0.0%)
1	B	0.26	0/2910	0.52	0/3937
1	E	0.25	0/2920	0.51	0/3951
1	F	0.26	0/2914	0.53	0/3943
2	D	0.27	0/1317	0.58	0/1783
2	Y	0.37	1/1429 (0.1%)	0.67	1/1933 (0.1%)
2	Z	0.47	3/1368 (0.2%)	0.70	4/1854 (0.2%)
All	All	0.33	7/15816 (0.0%)	0.57	7/21403 (0.0%)

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	F	0	1
2	D	0	2
2	Y	0	3
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	366	ARG	C-O	13.34	1.48	1.23
2	Z	519	LEU	CA-C	-7.32	1.33	1.52
1	A	176	HIS	N-CA	-7.30	1.31	1.46
2	Z	519	LEU	CA-CB	-7.24	1.37	1.53
2	Y	518	HIS	CA-C	-6.61	1.35	1.52
1	A	176	HIS	C-O	-5.89	1.12	1.23
2	Z	519	LEU	C-O	-5.14	1.13	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Z	519	LEU	C-N-CA	-7.67	102.54	121.70
2	Z	519	LEU	CB-CA-C	-7.56	95.84	110.20
1	A	367	ILE	CB-CA-C	-7.26	97.08	111.60
2	Z	630	PRO	N-CA-CB	5.98	110.48	103.30
1	A	-5	PRO	N-CA-CB	5.91	110.39	103.30
2	Y	622	LEU	CA-CB-CG	5.44	127.80	115.30
2	Z	519	LEU	N-CA-CB	-5.29	99.83	110.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	612	ARG	Peptide
2	D	642	TRP	Peptide
1	F	280	ARG	Peptide
2	Y	517	GLN	Mainchain
2	Y	522	PRO	Peptide
2	Y	526	ALA	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	2912	0	2944	65	0
1	B	2865	0	2913	48	0
1	E	2874	0	2921	33	0
1	F	2869	0	2916	41	0
2	D	1300	0	1283	52	0
2	Y	1409	0	1411	69	0
2	Z	1352	0	1318	37	0
All	All	15581	0	15706	307	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 10.

All (307) 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:Y:609:ARG:HD3	2:D:524:THR:HB	1.54	0.90
1:A:367:ILE:OXT	1:A:367:ILE:HG22	1.73	0.88
1:B:343:ASP:OD1	1:B:346:ARG:HD2	1.79	0.83
1:B:241:LYS:NZ	2:D:612:ARG:HG3	1.97	0.80
1:B:363:MET:HG3	2:Y:520:LEU:CD1	2.13	0.78
1:B:241:LYS:HZ1	2:D:612:ARG:HG3	1.49	0.76
1:A:283:ARG:HG3	1:A:367:ILE:HD12	1.67	0.76
1:B:363:MET:HG3	2:Y:520:LEU:HD13	1.67	0.75
1:A:248:VAL:HG13	2:Z:520:LEU:HD21	1.68	0.74
1:A:41:GLY:HA2	1:A:62:GLY:HA2	1.70	0.74
2:Y:556:THR:HG21	2:D:610:ALA:HB2	1.68	0.74
2:D:474:LEU:HB2	2:D:478:TYR:HB2	1.68	0.74
2:Z:487:LEU:HD23	2:Z:645:LEU:O	1.87	0.73
2:Y:652:THR:HG22	2:Z:643:VAL:HG11	1.70	0.72
1:A:150:GLN:O	1:A:150:GLN:HG2	1.88	0.72
2:D:600:ALA:HA	2:D:603:SER:HB3	1.71	0.71
2:Y:475:LEU:HD11	2:Z:647:LEU:HD13	1.72	0.70
2:Y:569:SER:OG	2:Y:609:ARG:NH1	2.19	0.70
2:Y:634:GLN:HG3	2:Y:638:GLY:HA2	1.75	0.69
1:E:152:ILE:HD11	2:Y:467:LEU:HB2	1.74	0.68
2:D:487:LEU:HG	2:D:645:LEU:HD22	1.76	0.67
2:D:525:PHE:HZ	2:D:559:VAL:HG13	1.59	0.67
2:Z:548:GLU:HB2	2:Z:561:ALA:HB3	1.76	0.67
1:A:66:PHE:HB2	1:F:152:ILE:HG12	1.77	0.66
1:B:46:LEU:HD13	1:B:55:ASP:HB3	1.78	0.66
2:D:616:LEU:HA	2:D:619:MET:HB2	1.78	0.66
2:Y:599:LEU:HD12	2:Y:601:THR:H	1.60	0.66
1:A:248:VAL:HG13	2:Z:520:LEU:CD2	2.27	0.65
1:F:280:ARG:NH1	1:F:322:ILE:HB	2.12	0.65
2:Z:477:ILE:HD11	2:Z:489:LEU:HD12	1.79	0.65
2:Z:493:HIS:HA	2:Z:496:ALA:HB3	1.78	0.65
1:A:163:VAL:O	1:A:191:ARG:HA	1.97	0.64
2:D:525:PHE:CZ	2:D:559:VAL:HG13	2.33	0.64
2:Y:600:ALA:HA	2:Y:603:SER:HB3	1.78	0.64
2:Y:566:LEU:HD23	2:Y:605:HIS:HB3	1.79	0.63
1:A:54:ILE:HG23	1:A:233:ILE:HG12	1.80	0.63
1:B:14:PRO:HB2	1:B:45:LEU:HD12	1.81	0.63
1:E:145:TYR:O	1:E:177:ARG:NH2	2.32	0.63
1:A:286:LEU:O	1:A:315:GLU:HA	1.99	0.63
1:B:261:ARG:HB2	1:B:337:MET:HG3	1.81	0.62
1:B:150:GLN:OE1	2:Y:612:ARG:NH1	2.31	0.62
2:Y:615:THR:O	2:Y:616:LEU:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:159:LEU:HD21	1:F:170:LEU:HB3	1.82	0.62
1:A:127:ALA:HB1	1:A:189:LEU:HD13	1.83	0.61
1:B:143:VAL:HG23	1:B:159:LEU:HD11	1.82	0.61
1:A:148:ALA:HB2	1:A:174:ASP:HA	1.83	0.61
1:F:259:LEU:HD11	1:F:264:LEU:HD22	1.80	0.61
2:D:479:ILE:HG23	2:D:490:ILE:HB	1.83	0.61
2:D:488:LEU:HD13	2:D:643:VAL:HG22	1.83	0.60
1:A:36:ILE:HD12	1:A:68:ILE:HD11	1.84	0.60
2:D:527:ALA:HB3	2:D:556:THR:HA	1.84	0.59
2:D:622:LEU:HD23	2:D:622:LEU:O	2.02	0.59
1:F:268:LEU:HB3	1:F:322:ILE:HD11	1.84	0.59
2:Y:488:LEU:HB3	2:Y:643:VAL:HG22	1.85	0.59
1:E:350:PHE:HB2	1:E:360:TYR:HB3	1.84	0.59
1:F:255:LYS:HB2	1:F:341:PHE:HB2	1.83	0.59
1:E:28:LEU:HG	2:Y:510:GLU:HG3	1.85	0.59
1:A:145:TYR:O	1:A:177:ARG:NH2	2.36	0.59
1:F:311:TYR:OH	1:F:313:GLY:O	2.12	0.59
1:F:15:LEU:HD11	1:F:75:PHE:CD2	2.39	0.58
2:D:479:ILE:HD11	2:D:619:MET:HB3	1.85	0.58
1:A:68:ILE:HG22	1:F:152:ILE:HG13	1.86	0.58
2:Y:632:SER:HB3	2:Y:642:TRP:HH2	1.69	0.58
2:Y:552:MET:HB2	2:Y:556:THR:HG23	1.85	0.58
1:A:248:VAL:HG13	2:Z:520:LEU:HD11	1.86	0.57
1:E:286:LEU:O	1:E:315:GLU:HA	2.05	0.57
2:D:535:LEU:HD12	2:D:557:LEU:HD13	1.85	0.57
1:A:300:GLN:O	1:B:96:ARG:NH2	2.37	0.57
2:Y:496:ALA:HA	2:Y:499:VAL:HG12	1.88	0.56
2:Y:474:LEU:HG	2:Y:480:LEU:HD22	1.87	0.56
2:Z:474:LEU:HG	2:Z:475:LEU:H	1.71	0.56
1:F:127:ALA:HB1	1:F:189:LEU:HD13	1.87	0.56
2:Y:520:LEU:HB3	2:Y:521:ILE:HG13	1.88	0.56
2:Y:527:ALA:HB3	2:Y:556:THR:HA	1.87	0.55
2:D:542:LEU:HD13	2:D:549:LEU:HD21	1.89	0.55
1:F:156:LEU:HD22	1:F:173:THR:HG23	1.89	0.55
1:E:127:ALA:HB1	1:E:189:LEU:HD13	1.88	0.55
1:E:152:ILE:CD1	2:Y:467:LEU:HB2	2.36	0.55
2:Y:639:ARG:NH2	2:Z:651:ASP:OD1	2.40	0.55
2:D:496:ALA:HA	2:D:499:VAL:HG12	1.89	0.54
2:Z:566:LEU:HD13	2:Z:574:LEU:HD22	1.88	0.54
1:A:15:LEU:HD11	1:A:75:PHE:CD2	2.43	0.54
2:D:566:LEU:HD22	2:D:574:LEU:HD21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:TYR:O	1:B:177:ARG:NH2	2.41	0.54
2:Y:479:ILE:HG23	2:Y:490:ILE:HB	1.89	0.54
2:D:514:LEU:HD13	2:D:545:PHE:HA	1.90	0.54
2:Z:487:LEU:HD21	2:Z:645:LEU:HD22	1.90	0.54
1:E:163:VAL:O	1:E:191:ARG:HA	2.08	0.54
2:Y:477:ILE:HD13	2:D:553:GLY:HA3	1.89	0.53
2:Y:581:GLU:HG2	2:Y:597:ARG:HG3	1.91	0.53
1:F:280:ARG:HB3	1:F:280:ARG:CZ	2.39	0.53
2:D:625:ASP:OD1	2:D:626:MET:N	2.41	0.53
2:D:486:SER:HB2	2:D:645:LEU:HD23	1.89	0.52
2:Y:609:ARG:HD3	2:D:524:THR:CB	2.35	0.52
2:Y:487:LEU:HD23	2:Z:474:LEU:HD22	1.90	0.52
1:A:52:ILE:HD12	1:A:199:LYS:HD3	1.91	0.52
2:D:599:LEU:HD12	2:D:601:THR:H	1.74	0.52
1:A:162:GLN:HE22	1:A:191:ARG:HH21	1.56	0.52
1:A:275:ALA:HB2	1:A:295:CYS:HB3	1.91	0.52
1:B:159:LEU:HD21	1:B:170:LEU:HB3	1.92	0.52
1:A:8:ARG:HD3	1:A:83:PRO:O	2.11	0.51
2:Z:600:ALA:O	2:Z:603:SER:OG	2.20	0.51
2:D:522:PRO:HB3	2:D:559:VAL:O	2.09	0.51
2:D:599:LEU:O	2:D:602:MET:N	2.43	0.51
1:B:139:MET:O	1:B:143:VAL:HG22	2.10	0.51
1:A:21:ILE:HD13	1:A:54:ILE:HG13	1.91	0.51
2:Z:492:MET:HG3	2:Z:493:HIS:CD2	2.45	0.51
1:B:121:VAL:HG22	1:B:234:VAL:HG11	1.93	0.51
1:F:272:SER:HB3	1:F:322:ILE:HD13	1.93	0.51
2:Y:614:LEU:HD22	2:Y:618:GLU:HG3	1.92	0.51
2:Z:524:THR:HG22	2:Z:558:ALA:HB2	1.92	0.51
2:Y:547:LEU:HG	2:Y:563:PRO:HD3	1.90	0.51
2:D:639:ARG:HG3	2:D:640:PRO:HD2	1.91	0.51
1:E:90:LEU:HB3	1:E:97:LEU:HD11	1.92	0.50
2:D:625:ASP:O	2:D:629:THR:OG1	2.28	0.50
1:A:156:LEU:HD22	1:A:173:THR:HG23	1.92	0.50
1:F:338:GLN:HB2	1:F:353:PRO:HG3	1.93	0.50
2:Y:480:LEU:HA	2:Y:488:LEU:O	2.10	0.50
2:Y:650:LEU:HA	2:Y:653:LEU:HD13	1.93	0.50
2:Y:477:ILE:HD11	2:Z:647:LEU:HD11	1.94	0.50
2:Z:529:HIS:CE1	2:Z:531:GLU:HA	2.46	0.50
2:Y:535:LEU:HD11	2:Y:549:LEU:HG	1.92	0.50
1:A:248:VAL:HG13	2:Z:520:LEU:CD1	2.42	0.50
1:A:3:ILE:HG12	1:A:90:LEU:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:PHE:HB2	1:B:360:TYR:HB3	1.93	0.49
2:Y:620:ASN:HA	2:Y:623:LEU:HB2	1.93	0.49
1:B:15:LEU:HD11	1:B:75:PHE:CD2	2.47	0.49
2:Y:494:ALA:O	2:Y:498:ARG:HG2	2.12	0.49
1:A:15:LEU:HD12	1:A:79:LEU:HD12	1.93	0.49
1:F:21:ILE:HD13	1:F:54:ILE:HG13	1.94	0.49
2:Y:607:SER:OG	2:Y:608:ILE:N	2.46	0.49
2:Y:598:ILE:HA	2:Y:602:MET:HB3	1.95	0.49
1:E:139:MET:O	1:E:143:VAL:HG22	2.12	0.49
2:Y:636:ASN:HD22	2:D:529:HIS:CE1	2.31	0.49
2:D:619:MET:O	2:D:623:LEU:HD23	2.12	0.49
2:Y:504:MET:HB3	2:Y:598:ILE:HD11	1.95	0.49
1:A:156:LEU:HD13	1:A:174:ASP:O	2.13	0.48
1:B:21:ILE:HG23	1:B:203:GLU:HG3	1.95	0.48
2:Y:471:ILE:HD13	2:Y:482:GLN:HB2	1.95	0.48
2:D:520:LEU:HD12	2:D:520:LEU:H	1.79	0.48
1:A:21:ILE:HA	1:A:199:LYS:HE2	1.96	0.48
1:F:69:THR:OG1	1:F:111:LEU:HB2	2.14	0.48
1:A:158:GLY:HA3	1:A:196:LEU:O	2.14	0.48
1:E:75:PHE:HE1	1:E:99:LEU:HD21	1.79	0.48
1:E:96:ARG:NH2	1:F:300:GLN:O	2.45	0.48
2:Y:523:VAL:HG22	2:Y:559:VAL:H	1.78	0.48
1:A:150:GLN:O	1:A:150:GLN:CG	2.61	0.48
1:B:38:GLY:O	1:B:65:ASP:HA	2.14	0.48
1:F:14:PRO:HB2	1:F:45:LEU:HD12	1.95	0.48
1:E:272:SER:HB3	1:E:322:ILE:HD13	1.95	0.47
2:Y:609:ARG:CD	2:D:524:THR:HB	2.35	0.47
2:D:488:LEU:HD22	2:D:643:VAL:HG13	1.95	0.47
1:A:365:MET:HB3	2:Z:517:GLN:OE1	2.15	0.47
1:F:28:LEU:HB2	1:F:31:LEU:HD12	1.95	0.47
1:A:248:VAL:HG22	2:Z:520:LEU:HD22	1.95	0.47
1:F:144:GLN:HG3	1:F:145:TYR:N	2.30	0.47
2:Y:468:GLY:HA2	2:Y:483:ALA:HB2	1.96	0.47
1:B:92:TRP:NE1	1:B:94:ASP:O	2.48	0.47
1:B:291:LEU:HB2	1:B:309:ILE:HD13	1.96	0.47
1:E:363:MET:HG3	1:E:364:PRO:HD2	1.96	0.47
2:Y:551:ASP:HA	2:Y:557:LEU:HD23	1.96	0.47
1:B:69:THR:HG1	1:B:111:LEU:HB2	1.79	0.47
2:Y:553:GLY:O	2:Y:556:THR:HG22	2.14	0.47
2:Y:604:CYS:SG	2:D:576:ARG:NH1	2.88	0.47
1:A:215:ILE:HD11	1:A:226:PHE:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:PHE:HE2	1:E:204:LEU:HD21	1.79	0.46
2:D:524:THR:HG22	2:D:556:THR:OG1	2.15	0.46
1:B:69:THR:OG1	1:B:111:LEU:HB2	2.14	0.46
1:F:98:THR:HG21	1:F:100:LYS:HE3	1.96	0.46
2:Y:479:ILE:HD11	2:Y:619:MET:HB3	1.97	0.46
2:Z:569:SER:OG	2:Z:570:ASP:N	2.48	0.46
1:A:18:PHE:HE2	1:A:45:LEU:HB2	1.81	0.46
2:Y:609:ARG:HG3	2:Y:610:ALA:H	1.80	0.46
1:A:99:LEU:HB2	1:A:106:PHE:HB2	1.97	0.46
2:Z:618:GLU:HA	2:Z:621:ALA:HB3	1.97	0.46
1:B:215:ILE:HD11	1:B:226:PHE:HB3	1.96	0.46
1:E:18:PHE:CE2	1:E:45:LEU:HB2	2.50	0.46
1:F:290:LEU:HD11	1:F:306:GLU:HB3	1.97	0.46
1:A:-3:GLY:HA2	1:A:93:ASP:OD1	2.16	0.46
2:Z:501:TYR:O	2:Z:504:MET:HB2	2.16	0.46
1:B:4:LEU:HD23	1:B:90:LEU:HD12	1.97	0.46
1:F:280:ARG:HH12	1:F:322:ILE:HB	1.81	0.46
2:Y:605:HIS:ND1	2:Y:606:GLY:O	2.49	0.46
1:F:8:ARG:HD3	1:F:83:PRO:O	2.16	0.45
2:Y:474:LEU:HD12	2:Y:480:LEU:HB3	1.97	0.45
2:Y:648:LYS:HA	2:Y:648:LYS:HD3	1.82	0.45
2:Z:521:ILE:O	2:Z:521:ILE:HG13	2.16	0.45
1:F:8:ARG:HD2	1:F:79:LEU:O	2.16	0.45
2:D:481:ALA:O	2:D:487:LEU:HA	2.17	0.45
1:A:178:LEU:HD13	1:A:248:VAL:HG11	1.97	0.45
1:B:148:ALA:HB2	1:B:174:ASP:HA	1.99	0.45
1:B:268:LEU:HD22	1:B:322:ILE:HG13	1.99	0.45
2:D:627:GLU:OE1	2:D:627:GLU:N	2.48	0.45
1:E:18:PHE:CZ	1:E:56:THR:HG22	2.51	0.45
2:Z:612:ARG:HD3	2:Z:612:ARG:HA	1.78	0.45
1:B:54:ILE:HG23	1:B:233:ILE:HG12	1.99	0.45
1:F:155:TYR:HA	1:F:238:ILE:HG21	1.99	0.45
1:F:268:LEU:HD23	1:F:293:VAL:HG11	1.97	0.45
1:A:18:PHE:HE1	1:A:54:ILE:HG22	1.80	0.45
1:A:139:MET:O	1:A:143:VAL:HG22	2.18	0.44
2:Z:472:ALA:H	2:Z:479:ILE:HG23	1.81	0.44
1:E:69:THR:OG1	1:E:111:LEU:HB2	2.17	0.44
1:E:99:LEU:HB2	1:E:106:PHE:HB2	2.00	0.44
1:F:352:VAL:HB	1:F:355:ASN:HB3	1.99	0.44
1:A:36:ILE:HG12	1:A:45:LEU:HD22	2.00	0.44
1:F:139:MET:O	1:F:143:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:581:GLU:HG2	2:D:597:ARG:HG2	1.99	0.44
1:A:35:LEU:HD12	1:A:68:ILE:O	2.17	0.44
1:A:159:LEU:HD21	1:A:170:LEU:HB3	2.00	0.44
1:B:340:ALA:HB3	1:B:349:LEU:HB3	1.98	0.44
2:Z:474:LEU:HD21	2:Z:477:ILE:HG23	2.00	0.44
2:D:612:ARG:NH2	2:D:614:LEU:HD11	2.32	0.44
1:A:8:ARG:HD2	1:A:79:LEU:O	2.18	0.44
1:B:5:GLN:HG2	1:B:87:LEU:HD11	2.00	0.44
1:E:35:LEU:HD12	1:E:68:ILE:O	2.17	0.44
1:B:284:LEU:HD23	1:B:320:PHE:HD2	1.83	0.44
1:E:261:ARG:NH1	1:E:329:LEU:O	2.49	0.44
1:B:352:VAL:HB	1:B:355:ASN:HB3	2.00	0.44
1:E:21:ILE:HA	1:E:199:LYS:HE2	1.99	0.44
2:Y:471:ILE:HG13	2:Y:480:LEU:HG	2.00	0.44
1:A:11:LEU:HG	1:A:59:PRO:HG3	1.99	0.43
1:E:54:ILE:HG23	1:E:233:ILE:HG12	2.00	0.43
2:D:470:ALA:HA	2:D:481:ALA:HA	2.00	0.43
2:Y:646:THR:HG23	2:Y:648:LYS:H	1.83	0.43
1:B:94:ASP:HB3	1:B:95:ASN:H	1.58	0.43
1:E:91:ASP:O	1:E:97:LEU:HD12	2.18	0.43
1:F:38:GLY:HA3	1:F:66:PHE:CE1	2.53	0.43
2:Y:508:ARG:HD3	2:Y:514:LEU:HD12	1.99	0.43
1:A:158:GLY:CA	1:A:196:LEU:O	2.66	0.43
1:E:297:ASN:HD21	1:E:301:GLU:HB2	1.82	0.43
2:D:566:LEU:HA	2:D:605:HIS:CE1	2.53	0.43
1:A:177:ARG:HD3	1:A:324:TYR:CD1	2.53	0.43
2:Y:538:HIS:O	2:Y:538:HIS:ND1	2.52	0.43
1:A:174:ASP:OD1	1:A:177:ARG:HG2	2.18	0.43
1:E:21:ILE:HG23	1:E:203:GLU:HG3	2.00	0.43
1:B:151:ASP:OD1	1:B:152:ILE:N	2.52	0.43
1:E:18:PHE:O	1:E:22:VAL:HG23	2.18	0.43
1:A:18:PHE:CE2	1:A:56:THR:HG22	2.54	0.43
1:A:82:LEU:HD23	1:B:270:ARG:HD3	2.01	0.43
1:B:136:PHE:HE2	1:B:204:LEU:HD21	1.84	0.43
1:F:160:LEU:HD11	1:F:193:GLU:HB2	2.01	0.43
2:Y:493:HIS:ND1	2:D:555:ASN:OD1	2.52	0.43
1:A:-4:ARG:HA	1:F:176:HIS:CE1	2.54	0.42
1:B:339:LEU:HB3	1:B:341:PHE:HE1	1.83	0.42
2:Y:547:LEU:HD13	2:Y:575:ALA:HA	2.00	0.42
2:D:569:SER:HB3	2:D:605:HIS:CD2	2.54	0.42
1:A:14:PRO:HB2	1:A:45:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:ILE:HG12	1:E:116:PHE:HD1	1.85	0.42
2:Y:570:ASP:OD1	2:Y:573:SER:OG	2.33	0.42
2:D:646:THR:O	2:D:646:THR:OG1	2.36	0.42
1:A:248:VAL:CG1	2:Z:520:LEU:HD11	2.49	0.42
2:Y:653:LEU:O	2:Z:640:PRO:HD2	2.19	0.42
1:A:164:GLU:OE1	1:A:169:ARG:NH2	2.45	0.42
1:A:268:LEU:HD23	1:A:293:VAL:HG11	2.02	0.42
1:A:128:THR:HG23	1:A:218:GLU:HG2	2.01	0.42
1:F:136:PHE:HE2	1:F:204:LEU:HD21	1.83	0.42
2:Z:487:LEU:HD22	2:Z:650:LEU:HD11	2.01	0.42
2:D:564:VAL:HG23	2:D:565:MET:HG3	2.01	0.42
1:E:15:LEU:HD11	1:E:75:PHE:CD2	2.54	0.42
2:Y:566:LEU:HD22	2:Y:574:LEU:HD21	2.01	0.42
2:D:535:LEU:HD13	2:D:557:LEU:HD22	2.02	0.42
2:D:608:ILE:HG21	2:D:612:ARG:HD3	2.01	0.42
1:B:255:LYS:HB2	1:B:341:PHE:HB2	2.02	0.42
2:Z:473:GLN:HA	2:Z:478:TYR:HA	2.02	0.42
1:B:35:LEU:HD12	1:B:68:ILE:O	2.20	0.42
1:F:215:ILE:HA	1:F:228:CYS:HB3	2.02	0.42
2:Z:530:GLU:HG2	2:Z:532:CYS:SG	2.60	0.42
2:D:490:ILE:HA	2:D:641:THR:O	2.20	0.42
1:A:92:TRP:CD2	1:F:152:ILE:HB	2.54	0.42
1:B:144:GLN:HG3	1:B:145:TYR:N	2.34	0.42
1:E:198:ARG:O	1:E:202:LEU:HG	2.19	0.42
2:Y:625:ASP:OD1	2:Y:626:MET:N	2.51	0.42
1:F:195:ILE:HG22	1:F:238:ILE:HD12	2.01	0.41
2:Y:501:TYR:CD1	2:Y:599:LEU:HA	2.55	0.41
1:A:273:ILE:HG21	1:B:78:ILE:HG13	2.02	0.41
2:Y:620:ASN:O	2:Y:624:ARG:HG2	2.20	0.41
1:A:38:GLY:HA3	1:A:66:PHE:CE2	2.55	0.41
1:A:139:MET:HE1	1:A:170:LEU:HG	2.03	0.41
1:F:15:LEU:HD12	1:F:79:LEU:HD12	2.00	0.41
1:F:318:VAL:HG11	1:F:341:PHE:HE2	1.85	0.41
2:Z:613:ARG:H	2:Z:613:ARG:HD3	1.85	0.41
1:A:36:ILE:HB	1:A:68:ILE:HG12	2.02	0.41
1:B:160:LEU:HD11	1:B:193:GLU:HB2	2.02	0.41
1:B:286:LEU:O	1:B:315:GLU:HA	2.21	0.41
1:B:178:LEU:HD13	1:B:248:VAL:HG11	2.01	0.41
1:B:156:LEU:HD22	1:B:173:THR:HG23	2.03	0.41
1:E:28:LEU:HD23	1:E:28:LEU:HA	1.91	0.41
2:D:480:LEU:HD12	2:D:487:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:480:LEU:HA	2:D:488:LEU:O	2.21	0.41
1:B:35:LEU:HD23	1:B:46:LEU:HD23	2.03	0.41
1:E:159:LEU:HD21	1:E:170:LEU:HD22	2.02	0.41
2:Z:581:GLU:HG3	2:Z:598:ILE:HD13	2.02	0.41
1:B:129:PHE:CE1	1:B:163:VAL:HG11	2.56	0.40
1:F:318:VAL:HG11	1:F:341:PHE:CE2	2.56	0.40
2:D:501:TYR:CZ	2:D:505:LYS:HD2	2.56	0.40
1:A:274:LEU:HB2	1:A:303:ALA:HB2	2.03	0.40
2:Y:472:ALA:HB3	2:Z:471:ILE:HG23	2.03	0.40
1:A:350:PHE:HB2	1:A:360:TYR:HB3	2.02	0.40
1:F:286:LEU:O	1:F:315:GLU:HA	2.20	0.40
2:Y:474:LEU:HB2	2:Y:478:TYR:HB2	2.03	0.40
2:Y:474:LEU:O	2:Y:475:LEU:HG	2.22	0.40
1:A:347:SER:HB3	1:A:361:ILE:HG23	2.04	0.40
2:Y:488:LEU:HD22	2:Y:643:VAL:CG1	2.51	0.40
1:A:13:LYS:HB3	1:A:14:PRO:HD3	2.02	0.40
1:B:220:LEU:HB2	1:B:223:GLN:HB2	2.04	0.40
1:E:347:SER:HB3	1:E:361:ILE:HG23	2.03	0.40
1:F:198:ARG:O	1:F:202:LEU:HG	2.22	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	372/387 (96%)	357 (96%)	15 (4%)	0	100	100
1	B	364/387 (94%)	352 (97%)	12 (3%)	0	100	100
1	E	365/387 (94%)	354 (97%)	11 (3%)	0	100	100
1	F	365/387 (94%)	352 (96%)	13 (4%)	0	100	100
2	D	170/220 (77%)	137 (81%)	32 (19%)	1 (1%)	22	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	Y	182/220 (83%)	132 (72%)	48 (26%)	2 (1%)	12 45
2	Z	183/220 (83%)	145 (79%)	37 (20%)	1 (0%)	25 59
All	All	2001/2208 (91%)	1829 (91%)	168 (8%)	4 (0%)	44 75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Y	616	LEU
2	D	526	ALA
2	Y	612	ARG
2	Z	629	THR

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	313/329 (95%)	311 (99%)	2 (1%)	84 91
1	B	311/329 (94%)	310 (100%)	1 (0%)	91 96
1	E	312/329 (95%)	312 (100%)	0	100 100
1	F	311/329 (94%)	310 (100%)	1 (0%)	91 96
2	D	131/180 (73%)	126 (96%)	5 (4%)	28 57
2	Y	148/180 (82%)	148 (100%)	0	100 100
2	Z	131/180 (73%)	128 (98%)	3 (2%)	45 69
All	All	1657/1856 (89%)	1645 (99%)	12 (1%)	81 89

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LYS
1	A	150	GLN
1	B	346	ARG
1	F	205	PHE

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Mol	Chain	Res	Type
2	Z	474	LEU
2	Z	613	ARG
2	Z	614	LEU
2	D	469	PHE
2	D	520	LEU
2	D	549	LEU
2	D	568	LYS
2	D	639	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	GLN
1	B	5	GLN
1	E	5	GLN
1	E	287	GLN
2	Y	515	GLN
2	Y	636	ASN
2	D	605	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	374/387 (96%)	-0.03	9 (2%) 59 41	67, 103, 130, 146	0
1	B	366/387 (94%)	-0.10	1 (0%) 90 82	74, 117, 152, 166	0
1	E	367/387 (94%)	-0.03	3 (0%) 82 67	82, 123, 159, 169	0
1	F	367/387 (94%)	-0.07	4 (1%) 77 59	71, 97, 125, 142	0
2	D	176/220 (80%)	0.84	22 (12%) 9 7	132, 161, 189, 202	0
2	Y	186/220 (84%)	0.68	21 (11%) 11 9	109, 147, 180, 192	0
2	Z	187/220 (85%)	0.58	10 (5%) 33 24	118, 166, 184, 203	0
All	All	2023/2208 (91%)	0.15	70 (3%) 47 32	67, 121, 173, 203	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	63	ALA	4.8
1	A	20	GLY	3.6
2	Y	607	SER	3.6
2	D	525	PHE	3.5
2	D	652	THR	3.4
2	Y	568	LYS	3.3
1	A	92	TRP	3.3
2	Z	496	ALA	3.3
1	E	19	THR	3.3
2	Z	608	ILE	3.2
2	D	644	LYS	3.2
2	D	645	LEU	3.1
2	Y	567	GLY	3.1
2	D	601	THR	3.1
2	Y	585	VAL	3.0
1	F	280	ARG	3.0
2	Y	608	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	521	ILE	3.0
2	D	649	GLU	3.0
2	D	608	ILE	3.0
2	D	487	LEU	2.9
1	A	94	ASP	2.8
2	Z	585	VAL	2.8
2	Z	565	MET	2.8
1	A	93	ASP	2.8
2	Y	614	LEU	2.8
2	Y	645	LEU	2.7
2	D	647	LEU	2.7
1	F	64	GLY	2.7
2	D	474	LEU	2.7
1	A	95	ASN	2.7
2	Y	653	LEU	2.7
2	Z	606	GLY	2.6
2	Z	474	LEU	2.6
1	E	5	GLN	2.6
2	Y	522	PRO	2.5
2	Y	487	LEU	2.5
1	B	367	ILE	2.5
1	A	25	LEU	2.5
1	A	19	THR	2.4
2	Y	467	LEU	2.4
1	F	281	GLY	2.4
2	D	628	ASN	2.4
2	Y	565	MET	2.3
2	Y	622	LEU	2.3
2	Z	467	LEU	2.3
2	Z	653	LEU	2.3
1	A	144	GLN	2.3
2	Y	586	GLY	2.3
2	D	602	MET	2.2
2	Y	643	VAL	2.2
2	D	622	LEU	2.2
2	Y	523	VAL	2.2
2	Y	524	THR	2.2
1	E	95	ASN	2.2
2	D	565	MET	2.1
2	D	528	SER	2.1
2	D	527	ALA	2.1
2	D	469	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	473	GLN	2.1
2	D	467	LEU	2.1
2	Y	555	ASN	2.1
2	Y	527	ALA	2.1
2	Y	521	ILE	2.1
2	Y	485	ASP	2.1
1	A	64	GLY	2.1
2	D	583	ALA	2.0
2	D	638	GLY	2.0
2	Z	464	LEU	2.0
2	Z	490	ILE	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.