



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:28 PM GMT

PDB ID : 5D17
Title : Structure of the C-terminal domain of TnsE at 2.85 resolution
Authors : Guarne, A.; Caron, J.J.
Deposited on : 2015-08-03
Resolution : 2.85 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
<http://wwpdb.org/validation/2016/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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

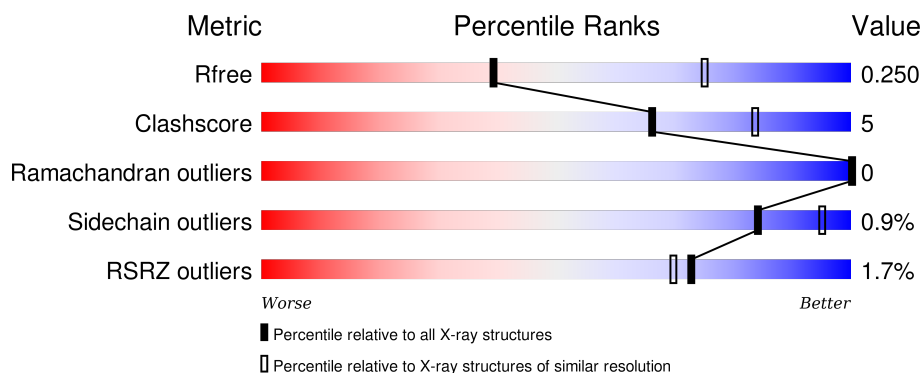
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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 $\leq 5\%$. 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	206	<div> <div></div> <div>66%11%23%</div> </div>
1	B	206	<div> <div></div> <div>65%11%23%</div> </div>
1	C	206	<div> <div></div> <div>66%11%23%</div> </div>
1	D	206	<div> <div></div> <div>68%8%24%</div> </div>
1	E	206	<div> <div></div> <div>70%6%23%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	206	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>64%</div><div>13%</div><div>23%</div></div></div>
1	G	206	<div><div><div></div><div></div><div></div></div><div><div></div><div>68%</div><div>8%</div><div>23%</div></div></div>
1	H	206	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>67%</div><div>8%</div><div>24%</div></div></div>
1	I	206	<div><div><div></div><div></div><div></div></div><div><div></div><div>68%</div><div>8%</div><div>23%</div></div></div>
1	K	206	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>66%</div><div>10%</div><div>24%</div></div></div>
1	L	206	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>67%</div><div>9%</div><div>23%</div></div></div>
1	M	206	<div><div><div></div><div></div><div></div></div><div><div></div><div>68%</div><div>9%</div><div>23%</div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14936 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 Transposon Tn7 transposition protein TnsE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	Se	0	6	0
			1252	793	217	237	2	3			
1	B	158	Total	C	N	O	S	Se	0	6	0
			1251	789	221	236	2	3			
1	C	158	Total	C	N	O	S	Se	0	6	0
			1266	797	226	238	2	3			
1	D	157	Total	C	N	O	S	Se	0	6	0
			1223	776	215	227	2	3			
1	E	158	Total	C	N	O	S	Se	0	6	0
			1234	782	217	230	2	3			
1	F	158	Total	C	N	O	S	Se	0	6	0
			1226	777	211	233	2	3			
1	G	158	Total	C	N	O	S	Se	0	6	0
			1242	788	216	233	2	3			
1	H	156	Total	C	N	O	S	Se	0	6	0
			1236	783	217	231	2	3			
1	I	158	Total	C	N	O	S	Se	0	6	0
			1269	799	228	237	2	3			
1	K	157	Total	C	N	O	S	Se	0	6	0
			1241	789	214	233	2	3			
1	L	158	Total	C	N	O	S	Se	0	6	0
			1209	771	209	224	2	3			
1	M	159	Total	C	N	O	S	Se	0	6	0
			1264	796	224	239	2	3			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	341	MSE	-	initiating methionine	UNP P05845
A	539	LEU	-	expression tag	UNP P05845
A	540	GLU	-	expression tag	UNP P05845
A	541	HIS	-	expression tag	UNP P05845
A	542	HIS	-	expression tag	UNP P05845

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Chain	Residue	Modelled	Actual	Comment	Reference
A	543	HIS	-	expression tag	UNP P05845
A	544	HIS	-	expression tag	UNP P05845
A	545	HIS	-	expression tag	UNP P05845
A	546	HIS	-	expression tag	UNP P05845
B	341	MSE	-	initiating methionine	UNP P05845
B	539	LEU	-	expression tag	UNP P05845
B	540	GLU	-	expression tag	UNP P05845
B	541	HIS	-	expression tag	UNP P05845
B	542	HIS	-	expression tag	UNP P05845
B	543	HIS	-	expression tag	UNP P05845
B	544	HIS	-	expression tag	UNP P05845
B	545	HIS	-	expression tag	UNP P05845
B	546	HIS	-	expression tag	UNP P05845
C	341	MSE	-	initiating methionine	UNP P05845
C	539	LEU	-	expression tag	UNP P05845
C	540	GLU	-	expression tag	UNP P05845
C	541	HIS	-	expression tag	UNP P05845
C	542	HIS	-	expression tag	UNP P05845
C	543	HIS	-	expression tag	UNP P05845
C	544	HIS	-	expression tag	UNP P05845
C	545	HIS	-	expression tag	UNP P05845
C	546	HIS	-	expression tag	UNP P05845
D	341	MSE	-	initiating methionine	UNP P05845
D	539	LEU	-	expression tag	UNP P05845
D	540	GLU	-	expression tag	UNP P05845
D	541	HIS	-	expression tag	UNP P05845
D	542	HIS	-	expression tag	UNP P05845
D	543	HIS	-	expression tag	UNP P05845
D	544	HIS	-	expression tag	UNP P05845
D	545	HIS	-	expression tag	UNP P05845
D	546	HIS	-	expression tag	UNP P05845
E	341	MSE	-	initiating methionine	UNP P05845
E	539	LEU	-	expression tag	UNP P05845
E	540	GLU	-	expression tag	UNP P05845
E	541	HIS	-	expression tag	UNP P05845
E	542	HIS	-	expression tag	UNP P05845
E	543	HIS	-	expression tag	UNP P05845
E	544	HIS	-	expression tag	UNP P05845
E	545	HIS	-	expression tag	UNP P05845
E	546	HIS	-	expression tag	UNP P05845
F	341	MSE	-	initiating methionine	UNP P05845
F	539	LEU	-	expression tag	UNP P05845

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Chain	Residue	Modelled	Actual	Comment	Reference
F	540	GLU	-	expression tag	UNP P05845
F	541	HIS	-	expression tag	UNP P05845
F	542	HIS	-	expression tag	UNP P05845
F	543	HIS	-	expression tag	UNP P05845
F	544	HIS	-	expression tag	UNP P05845
F	545	HIS	-	expression tag	UNP P05845
F	546	HIS	-	expression tag	UNP P05845
G	341	MSE	-	initiating methionine	UNP P05845
G	539	LEU	-	expression tag	UNP P05845
G	540	GLU	-	expression tag	UNP P05845
G	541	HIS	-	expression tag	UNP P05845
G	542	HIS	-	expression tag	UNP P05845
G	543	HIS	-	expression tag	UNP P05845
G	544	HIS	-	expression tag	UNP P05845
G	545	HIS	-	expression tag	UNP P05845
G	546	HIS	-	expression tag	UNP P05845
H	341	MSE	-	initiating methionine	UNP P05845
H	539	LEU	-	expression tag	UNP P05845
H	540	GLU	-	expression tag	UNP P05845
H	541	HIS	-	expression tag	UNP P05845
H	542	HIS	-	expression tag	UNP P05845
H	543	HIS	-	expression tag	UNP P05845
H	544	HIS	-	expression tag	UNP P05845
H	545	HIS	-	expression tag	UNP P05845
H	546	HIS	-	expression tag	UNP P05845
I	341	MSE	-	initiating methionine	UNP P05845
I	539	LEU	-	expression tag	UNP P05845
I	540	GLU	-	expression tag	UNP P05845
I	541	HIS	-	expression tag	UNP P05845
I	542	HIS	-	expression tag	UNP P05845
I	543	HIS	-	expression tag	UNP P05845
I	544	HIS	-	expression tag	UNP P05845
I	545	HIS	-	expression tag	UNP P05845
I	546	HIS	-	expression tag	UNP P05845
K	341	MSE	-	initiating methionine	UNP P05845
K	539	LEU	-	expression tag	UNP P05845
K	540	GLU	-	expression tag	UNP P05845
K	541	HIS	-	expression tag	UNP P05845
K	542	HIS	-	expression tag	UNP P05845
K	543	HIS	-	expression tag	UNP P05845
K	544	HIS	-	expression tag	UNP P05845
K	545	HIS	-	expression tag	UNP P05845

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Chain	Residue	Modelled	Actual	Comment	Reference
K	546	HIS	-	expression tag	UNP P05845
L	341	MSE	-	initiating methionine	UNP P05845
L	539	LEU	-	expression tag	UNP P05845
L	540	GLU	-	expression tag	UNP P05845
L	541	HIS	-	expression tag	UNP P05845
L	542	HIS	-	expression tag	UNP P05845
L	543	HIS	-	expression tag	UNP P05845
L	544	HIS	-	expression tag	UNP P05845
L	545	HIS	-	expression tag	UNP P05845
L	546	HIS	-	expression tag	UNP P05845
M	341	MSE	-	initiating methionine	UNP P05845
M	539	LEU	-	expression tag	UNP P05845
M	540	GLU	-	expression tag	UNP P05845
M	541	HIS	-	expression tag	UNP P05845
M	542	HIS	-	expression tag	UNP P05845
M	543	HIS	-	expression tag	UNP P05845
M	544	HIS	-	expression tag	UNP P05845
M	545	HIS	-	expression tag	UNP P05845
M	546	HIS	-	expression tag	UNP P05845

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O 1 1	0	0
2	B	1	Total O 1 1	0	0
2	C	1	Total O 1 1	0	0
2	D	1	Total O 1 1	0	0
2	E	2	Total O 2 2	0	0
2	F	1	Total O 1 1	0	0
2	G	8	Total O 8 8	0	0
2	H	2	Total O 2 2	0	0
2	I	2	Total O 2 2	0	0
2	K	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	1	Total	O	0	0
			1	1		
2	M	2	Total	O	0	0
			2	2		

3 Residue-property plots [i](#)

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: Transposon Tn7 transposition protein TnsE

Chain A: 



- Molecule 1: Transposon Tn7 transposition protein TnsE

Chain B: 



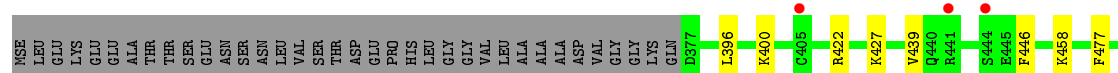
- Molecule 1: Transposon Tn7 transposition protein TnsE

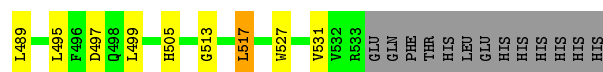
Chain C: 



- Molecule 1: Transposon Tn7 transposition protein TnsE

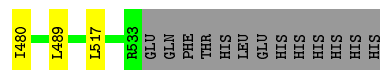
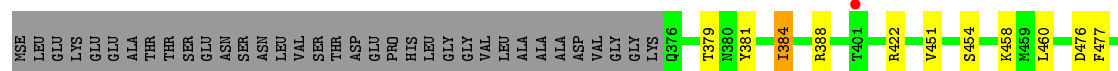
Chain D: 





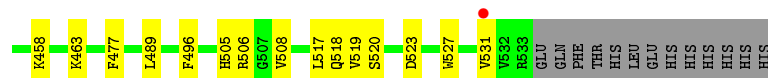
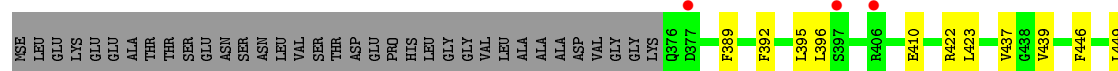
- Molecule 1: Transposon Tn7 transposition protein TnsE

Chain E: 70% 6% 23%



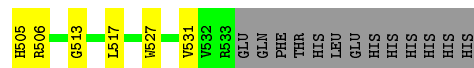
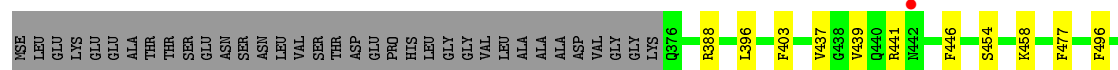
- Molecule 1: Transposon Tn7 transposition protein TnsE

Chain F: 2% 64% 13% 23%



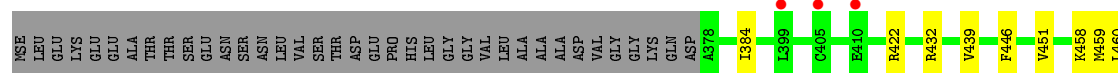
- Molecule 1: Transposon Tn7 transposition protein TnsE

Chain G: 68% 8% 23%



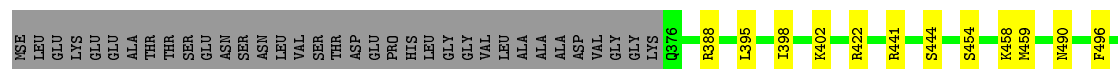
- Molecule 1: Transposon Tn7 transposition protein TnsE

Chain H: 2% 67% 8% 24%



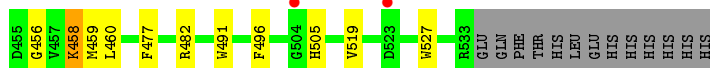
- Molecule 1: Transposon Tn7 transposition protein TnsE

Chain I: 68% 8% 23%

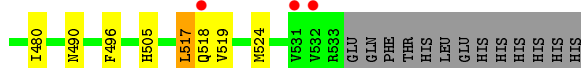




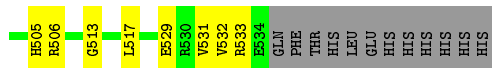
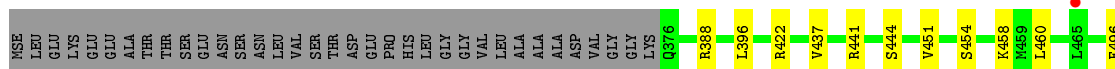
- Molecule 1: Transposon Tn7 transposition protein TnsE



- Molecule 1: Transposon Tn7 transposition protein TnsE



- Molecule 1: Transposon Tn7 transposition protein TnsE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.33Å 87.12Å 141.62Å 90.00° 95.01° 90.00°	Depositor
Resolution (Å)	39.75 – 2.85 43.21 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.75-2.85) 92.5 (43.21-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.221 , 0.251 0.222 , 0.250	Depositor DCC
R_{free} test set	3703 reflections (3.02%)	DCC
Wilson B-factor (Å ²)	68.4	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 66218 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14936	wwPDB-VP
Average B, all atoms (Å ²)	87.0	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 41.25 % 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 2.4261e-04. 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, 0.375 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	0.22	0/1272	0.41	0/1718
1	B	0.22	0/1271	0.41	0/1715
1	C	0.21	0/1285	0.42	0/1733
1	D	0.23	0/1243	0.49	2/1680 (0.1%)
1	E	0.22	0/1254	0.42	0/1695
1	F	0.25	0/1246	0.43	0/1686
1	G	0.22	0/1262	0.41	0/1704
1	H	0.21	0/1256	0.42	0/1695
1	I	0.22	0/1289	0.42	0/1737
1	K	0.22	0/1260	0.41	0/1699
1	L	0.22	0/1229	0.48	1/1664 (0.1%)
1	M	0.21	0/1284	0.42	0/1733
All	All	0.22	0/15151	0.43	3/20459 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	517	LEU	CB-CG-CD1	-7.38	98.45	111.00
1	D	517	LEU	CA-CB-CG	6.23	129.63	115.30
1	D	517	LEU	CB-CG-CD1	-6.02	100.77	111.00

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	1252	0	1200	16	0
1	B	1251	0	1208	16	0
1	C	1266	0	1230	15	0
1	D	1223	0	1177	14	0
1	E	1234	0	1183	11	0
1	F	1226	0	1157	21	0
1	G	1242	0	1197	11	0
1	H	1236	0	1200	16	0
1	I	1269	0	1243	12	0
1	K	1241	0	1209	15	0
1	L	1209	0	1151	13	0
1	M	1264	0	1221	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
2	G	8	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	2	0	0	0	0
All	All	14936	0	14376	143	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 (143) 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:F:506:ARG:NH2	1:F:531:VAL:O	2.10	0.84
1:G:517:LEU:HB2	1:H:518:GLN:HE21	1.43	0.82
1:I:422:ARG:HH22	1:K:458[B]:LYS:HB2	1.51	0.75
1:F:517:LEU:HG	1:F:518:GLN:N	2.03	0.73
1:I:459[A]:MSE:HE1	1:I:490:ASN:HA	1.71	0.72
1:A:422:ARG:NH2	1:E:458[B]:LYS:O	2.22	0.72
1:B:451:VAL:HB	1:B:460[B]:LEU:HD11	1.72	0.72
1:A:422:ARG:NH1	1:E:489:LEU:O	2.22	0.71
1:L:459[A]:MSE:HE1	1:L:490:ASN:HA	1.72	0.71
1:C:422:ARG:HH22	1:D:458[B]:LYS:HB2	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459[B]:MSE:HE1	1:C:514:LEU:HB3	1.73	0.70
1:B:458[B]:LYS:O	1:F:422:ARG:NH2	2.24	0.70
1:I:458[B]:LYS:HB2	1:K:422:ARG:HH22	1.57	0.70
1:M:506:ARG:NH1	1:M:531:VAL:O	2.27	0.68
1:H:451:VAL:HB	1:H:460[B]:LEU:HD11	1.75	0.67
1:D:517:LEU:HD21	1:F:518:GLN:HA	1.78	0.66
1:K:456:GLY:O	1:K:458[A]:LYS:NZ	2.29	0.66
1:K:451:VAL:HB	1:K:459[A]:MSE:HG3	1.79	0.64
1:B:402:LYS:NZ	1:B:525:GLU:OE2	2.31	0.64
1:I:398:ILE:HG23	1:I:402:LYS:HD2	1.78	0.63
1:D:517:LEU:HD11	1:F:517:LEU:C	2.19	0.63
1:C:497:ASP:OD1	1:C:505:HIS:NE2	2.28	0.63
1:B:489:LEU:O	1:F:422:ARG:NH1	2.33	0.62
1:H:489:LEU:O	1:M:422:ARG:NH1	2.30	0.61
1:I:506:ARG:NH1	1:I:531:VAL:O	2.31	0.61
1:F:517:LEU:HG	1:F:518:GLN:H	1.67	0.60
1:D:497:ASP:OD1	1:D:505:HIS:NE2	2.30	0.58
1:I:422:ARG:NH2	1:K:458[B]:LYS:HB2	2.18	0.58
1:H:459[A]:MSE:HE1	1:H:490:ASN:HA	1.86	0.56
1:A:458[B]:LYS:HB2	1:E:422:ARG:HH22	1.70	0.56
1:B:441:ARG:NH2	1:B:532:VAL:HB	2.21	0.56
1:C:458[B]:LYS:HB2	1:D:422:ARG:HH22	1.71	0.56
1:K:519:VAL:O	1:L:517:LEU:HD11	2.06	0.55
1:A:422:ARG:HH22	1:E:460[B]:LEU:HD23	1.71	0.54
1:A:451:VAL:HB	1:A:459[A]:MSE:HG3	1.89	0.54
1:M:451:VAL:HB	1:M:460[B]:LEU:HD11	1.90	0.53
1:E:451:VAL:HB	1:E:460[B]:LEU:HD11	1.90	0.53
1:H:508:VAL:HG21	1:H:531:VAL:HA	1.90	0.53
1:H:528:ALA:O	1:H:531:VAL:HG22	2.09	0.53
1:G:396:LEU:HD11	1:G:437:VAL:HG21	1.91	0.52
1:A:518:GLN:HG3	1:C:512:LYS:O	2.09	0.52
1:M:441:ARG:O	1:M:444:SER:OG	2.23	0.52
1:I:441:ARG:O	1:I:444:SER:OG	2.18	0.52
1:F:508:VAL:HG21	1:F:531:VAL:HA	1.92	0.52
1:A:458[B]:LYS:HB2	1:E:422:ARG:NH2	2.25	0.52
1:I:388:ARG:HG2	1:I:454:SER:HB3	1.92	0.51
1:A:496:PHE:HB3	1:A:505:HIS:CD2	2.45	0.51
1:M:513:GLY:O	1:M:517:LEU:HG	2.09	0.51
1:F:520:SER:OG	1:F:523:ASP:OD1	2.29	0.51
1:B:459[A]:MSE:HE1	1:B:490:ASN:HA	1.93	0.51
1:F:389:PHE:HB3	1:F:392:PHE:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:458[B]:LYS:HB2	1:K:422:ARG:NH2	2.24	0.50
1:G:513:GLY:O	1:G:517:LEU:HG	2.11	0.50
1:H:458[B]:LYS:HB2	1:M:422:ARG:NH2	2.27	0.50
1:C:422:ARG:NH2	1:D:458[B]:LYS:HB2	2.26	0.49
1:L:517:LEU:HD12	1:L:518:GLN:H	1.76	0.49
1:M:496:PHE:HB3	1:M:505:HIS:CD2	2.46	0.49
1:B:459[B]:MSE:HE1	1:B:514:LEU:HD23	1.94	0.49
1:G:388:ARG:HG2	1:G:454:SER:HB3	1.93	0.49
1:I:496:PHE:HB3	1:I:505:HIS:CD2	2.48	0.49
1:A:396:LEU:HD11	1:A:437:VAL:HG21	1.94	0.48
1:G:458[B]:LYS:HB2	1:L:422:ARG:HH22	1.78	0.48
1:E:388:ARG:HG2	1:E:454:SER:HB3	1.95	0.48
1:M:388:ARG:HG2	1:M:454:SER:HB3	1.96	0.48
1:L:519:VAL:HG11	1:L:524:MSE:SE	2.64	0.48
1:B:506:ARG:NH1	1:B:531:VAL:O	2.46	0.48
1:K:496:PHE:HB3	1:K:505:HIS:CD2	2.49	0.48
1:G:496:PHE:HB3	1:G:505:HIS:CD2	2.48	0.48
1:K:397:SER:HA	1:K:400:LYS:HE2	1.96	0.48
1:K:395:LEU:HD22	1:K:527:TRP:CZ2	2.48	0.47
1:B:528:ALA:O	1:B:531:VAL:HG22	2.15	0.47
1:K:389:PHE:HB3	1:K:392:PHE:HB3	1.96	0.46
1:L:476:ASP:O	1:L:480:ILE:HG13	2.15	0.46
1:C:458[B]:LYS:HB2	1:D:422:ARG:NH2	2.31	0.46
1:M:441:ARG:NH2	1:M:532:VAL:HB	2.30	0.46
1:F:527:TRP:O	1:F:531:VAL:HG23	2.15	0.46
1:B:422:ARG:HH12	1:F:458[B]:LYS:HB2	1.81	0.46
1:E:517:LEU:HA	1:F:517:LEU:HD13	1.97	0.46
1:H:518:GLN:OE1	1:I:520:SER:HB3	2.16	0.45
1:K:458[A]:LYS:H	1:K:458[A]:LYS:HG2	1.51	0.45
1:H:422:ARG:HH22	1:M:458[B]:LYS:N	2.15	0.45
1:A:449:LEU:HB2	1:A:463:LYS:HB3	1.98	0.45
1:C:460[B]:LEU:O	1:C:510:HIS:ND1	2.47	0.45
1:M:396:LEU:HD11	1:M:437:VAL:HG21	1.98	0.45
1:D:495:LEU:O	1:D:499:LEU:HG	2.16	0.45
1:A:406:ARG:HD3	1:A:440:GLN:OE1	2.17	0.45
1:L:411:GLU:HG3	1:L:436:ALA:HB3	1.99	0.44
1:H:496:PHE:HB3	1:H:505:HIS:CD2	2.51	0.44
1:C:388:ARG:HG2	1:C:454:SER:HB3	1.99	0.44
1:A:441:ARG:O	1:A:444:SER:OG	2.22	0.44
1:L:496:PHE:HB3	1:L:505:HIS:CD2	2.52	0.44
1:H:422:ARG:NH1	1:M:458[B]:LYS:O	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:423:LEU:HB3	1:F:489:LEU:HG	1.99	0.44
1:M:529:GLU:O	1:M:533:ARG:HG2	2.17	0.44
1:D:489:LEU:HA	1:D:489:LEU:HD23	1.86	0.44
1:E:381:TYR:HB3	1:E:384:ILE:HD11	2.00	0.44
1:C:440:GLN:HG3	1:C:445:GLU:HG2	2.00	0.44
1:G:458[B]:LYS:HB2	1:L:422:ARG:NH2	2.33	0.43
1:C:405:CYS:SG	1:C:441:ARG:HD2	2.58	0.43
1:G:506:ARG:NH1	1:G:531:VAL:O	2.50	0.43
1:G:439:VAL:HB	1:G:446:PHE:CE1	2.53	0.43
1:C:395:LEU:HD22	1:C:527:TRP:CZ2	2.53	0.43
1:G:403:PHE:HD2	1:G:441:ARG:HH12	1.67	0.43
1:L:451:VAL:HB	1:L:460[B]:LEU:HD11	2.00	0.43
1:F:410:GLU:HG2	1:F:437:VAL:HG22	2.01	0.43
1:C:456:GLY:HA3	1:D:427:LYS:HE3	2.00	0.43
1:K:379:THR:HB	1:K:381:TYR:CZ	2.54	0.43
1:F:496:PHE:HB3	1:F:505:HIS:CD2	2.54	0.43
1:D:396:LEU:O	1:D:400:LYS:HG3	2.18	0.43
1:A:459[B]:MSE:SE	1:A:514:LEU:HD23	2.69	0.43
1:B:496:PHE:HB3	1:B:505:HIS:CD2	2.54	0.43
1:D:527:TRP:O	1:D:531:VAL:HG23	2.19	0.42
1:F:449:LEU:HB2	1:F:463:LYS:HB3	2.02	0.42
1:A:450:GLU:OE1	1:A:510:HIS:NE2	2.47	0.42
1:L:519:VAL:HG12	1:L:524:MSE:HG2	2.02	0.42
1:F:396:LEU:HD11	1:F:437:VAL:HG21	2.01	0.42
1:K:388:ARG:HG2	1:K:454:SER:HB3	2.01	0.42
1:L:388:ARG:HG2	1:L:454:SER:HB3	2.02	0.42
1:L:439:VAL:HB	1:L:446:PHE:CE1	2.55	0.42
1:F:518:GLN:NE2	1:F:519:VAL:O	2.43	0.41
1:H:422:ARG:NH1	1:M:460[B]:LEU:HD23	2.34	0.41
1:G:527:TRP:O	1:G:531:VAL:HG23	2.20	0.41
1:B:394:GLU:O	1:B:398:ILE:HG13	2.20	0.41
1:F:395:LEU:HD22	1:F:527:TRP:CZ2	2.55	0.41
1:F:439:VAL:HB	1:F:446:PHE:CE1	2.55	0.41
1:E:476:ASP:O	1:E:480:ILE:HG13	2.20	0.41
1:C:408:LEU:HD11	1:C:440:GLN:HB2	2.02	0.41
1:A:388:ARG:HG2	1:A:454:SER:HB3	2.01	0.41
1:D:439:VAL:HB	1:D:446:PHE:CE1	2.56	0.41
1:E:379:THR:HB	1:E:381:TYR:CZ	2.56	0.41
1:K:460[B]:LEU:HD12	1:K:491:TRP:CE2	2.55	0.41
1:H:458[B]:LYS:HB2	1:M:422:ARG:HH22	1.84	0.41
1:B:508:VAL:HG21	1:B:531:VAL:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:VAL:HB	1:B:446:PHE:CE1	2.56	0.41
1:H:432:ARG:NE	1:H:489:LEU:HD11	2.36	0.41
1:H:439:VAL:HB	1:H:446:PHE:CE1	2.56	0.41
1:H:489:LEU:HA	1:H:489:LEU:HD23	1.92	0.40
1:A:379:THR:HB	1:A:381:TYR:CZ	2.56	0.40
1:D:513:GLY:O	1:D:517:LEU:HB3	2.21	0.40
1:I:395:LEU:HD22	1:I:527:TRP:CE2	2.57	0.40
1:C:400:LYS:HD3	1:C:407:VAL:HG23	2.02	0.40
1:B:489:LEU:HD23	1:B:489:LEU:HA	1.89	0.40
1:B:399:LEU:HD11	1:B:531:VAL:HG21	2.04	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	163/206 (79%)	160 (98%)	3 (2%)	0	100	100
1	B	162/206 (79%)	161 (99%)	1 (1%)	0	100	100
1	C	162/206 (79%)	159 (98%)	3 (2%)	0	100	100
1	D	161/206 (78%)	158 (98%)	3 (2%)	0	100	100
1	E	162/206 (79%)	159 (98%)	3 (2%)	0	100	100
1	F	162/206 (79%)	161 (99%)	1 (1%)	0	100	100
1	G	162/206 (79%)	161 (99%)	1 (1%)	0	100	100
1	H	160/206 (78%)	159 (99%)	1 (1%)	0	100	100
1	I	162/206 (79%)	159 (98%)	3 (2%)	0	100	100
1	K	161/206 (78%)	156 (97%)	5 (3%)	0	100	100
1	L	162/206 (79%)	161 (99%)	1 (1%)	0	100	100
1	M	163/206 (79%)	162 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1942/2472 (79%)	1916 (99%)	26 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	129/174 (74%)	128 (99%)	1 (1%)	86	96
1	B	131/174 (75%)	128 (98%)	3 (2%)	58	85
1	C	134/174 (77%)	133 (99%)	1 (1%)	88	96
1	D	125/174 (72%)	124 (99%)	1 (1%)	86	96
1	E	126/174 (72%)	124 (98%)	2 (2%)	70	90
1	F	124/174 (71%)	123 (99%)	1 (1%)	86	96
1	G	128/174 (74%)	127 (99%)	1 (1%)	86	96
1	H	129/174 (74%)	128 (99%)	1 (1%)	86	96
1	I	135/174 (78%)	135 (100%)	0	100	100
1	K	130/174 (75%)	126 (97%)	4 (3%)	47	79
1	L	121/174 (70%)	121 (100%)	0	100	100
1	M	133/174 (76%)	133 (100%)	0	100	100
All	All	1545/2088 (74%)	1530 (99%)	15 (1%)	84	94

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	477	PHE
1	B	459[A]	MSE
1	B	459[B]	MSE
1	B	477	PHE
1	C	489	LEU
1	D	477	PHE

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Mol	Chain	Res	Type
1	E	384	ILE
1	E	477	PHE
1	F	477	PHE
1	G	477	PHE
1	H	384	ILE
1	K	458[A]	LYS
1	K	458[B]	LYS
1	K	477	PHE
1	K	482	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	518	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	157/206 (76%)	-0.00	1 (0%) 90 89	52, 79, 120, 142	0
1	B	156/206 (75%)	0.00	3 (1%) 70 66	54, 87, 138, 157	0
1	C	156/206 (75%)	0.17	4 (2%) 59 54	55, 88, 136, 154	0
1	D	155/206 (75%)	0.07	3 (1%) 70 66	53, 93, 132, 144	0
1	E	156/206 (75%)	-0.05	1 (0%) 90 89	59, 95, 132, 147	0
1	F	156/206 (75%)	0.15	4 (2%) 59 54	59, 101, 140, 157	0
1	G	156/206 (75%)	-0.10	1 (0%) 90 89	49, 72, 99, 126	0
1	H	154/206 (74%)	0.11	5 (3%) 51 44	51, 86, 125, 134	0
1	I	156/206 (75%)	0.01	0 100 100	42, 70, 111, 128	0
1	K	155/206 (75%)	0.08	3 (1%) 70 66	41, 84, 127, 147	0
1	L	156/206 (75%)	0.16	5 (3%) 51 44	64, 112, 154, 175	0
1	M	157/206 (76%)	-0.13	1 (0%) 90 89	44, 75, 114, 131	0
All	All	1870/2472 (75%)	0.04	31 (1%) 73 70	41, 85, 134, 175	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	519	VAL	3.5
1	L	531	VAL	3.5
1	H	519	VAL	3.4
1	F	531	VAL	3.3
1	M	465	LEU	3.1
1	C	447	VAL	3.0
1	L	399	LEU	2.9
1	E	401	THR	2.9
1	G	442	ASN	2.6
1	C	532	VAL	2.6
1	H	399	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	397	SER	2.6
1	C	498	GLN	2.5
1	L	532	VAL	2.5
1	L	518	GLN	2.5
1	B	376	GLN	2.4
1	K	523	ASP	2.3
1	F	377	ASP	2.3
1	C	446	PHE	2.2
1	H	410	GLU	2.2
1	L	440	GLN	2.1
1	D	444	SER	2.1
1	A	406	ARG	2.1
1	H	405	CYS	2.1
1	D	405	CYS	2.1
1	B	518	GLN	2.1
1	K	504	GLY	2.0
1	K	405	CYS	2.0
1	F	406	ARG	2.0
1	D	441	ARG	2.0
1	H	518	GLN	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 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.