



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:10 PM GMT

PDB ID : 4WWU  
Title : Structure of Mex67:Mtr2  
Authors : Aibara, S.; Valkov, E.; Stewart, M.  
Deposited on : 2014-11-12  
Resolution : 3.30 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

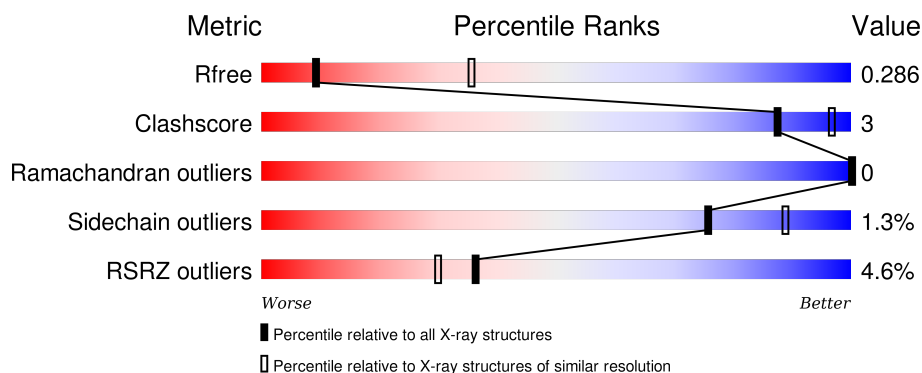
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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  $\geq 3$ , 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	488	<div> <div>6%</div> <div>11% •</div> <div>85%</div> </div>
1	B	488	<div> <div>%</div> <div>65%</div> <div>6%</div> <div>29%</div> </div>
1	D	488	<div> <div>6%</div> <div>13% •</div> <div>86%</div> </div>
1	E	488	<div> <div>66%</div> <div>6%</div> <div>28%</div> </div>
1	G	488	<div> <div>13% •</div> <div>86%</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	488	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>68%</div><div>6%</div><div>26%</div></div></div>
1	J	488	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>14%</div><div>85%</div><div></div></div></div>
1	K	488	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>68%</div><div>6%</div><div>27%</div></div></div>
2	C	184	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>85%</div><div></div><div>10%</div></div></div>
2	F	184	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>83%</div><div>6%</div><div>11%</div></div></div>
2	I	184	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>77%</div><div>10%</div><div>13%</div></div></div>
2	L	184	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>80%</div><div>8%</div><div>12%</div></div></div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 37509 atoms, of which 18712 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 mRNA export factor MEX67.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	71	Total	C	H	N	O	S	0	0	0
			1119	358	555	100	104	2			
1	B	347	Total	C	H	N	O	S	0	0	0
			5594	1776	2805	469	534	10			
1	D	69	Total	C	H	N	O	S	0	0	0
			1099	350	551	98	98	2			
1	E	349	Total	C	H	N	O	S	0	0	0
			5621	1787	2817	470	537	10			
1	G	69	Total	C	H	N	O	S	0	0	0
			1099	350	551	98	98	2			
1	H	363	Total	C	H	N	O	S	0	0	0
			5829	1852	2916	489	562	10			
1	J	71	Total	C	H	N	O	S	0	0	0
			1119	358	555	100	104	2			
1	K	358	Total	C	H	N	O	S	0	0	0
			5749	1827	2874	484	554	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q99257
A	93	ASP	ASN	conflict	UNP Q99257
B	0	SER	-	expression tag	UNP Q99257
B	93	ASP	ASN	conflict	UNP Q99257
D	0	SER	-	expression tag	UNP Q99257
D	93	ASP	ASN	conflict	UNP Q99257
E	0	SER	-	expression tag	UNP Q99257
E	93	ASP	ASN	conflict	UNP Q99257
G	0	SER	-	expression tag	UNP Q99257
G	93	ASP	ASN	conflict	UNP Q99257
H	0	SER	-	expression tag	UNP Q99257
H	93	ASP	ASN	conflict	UNP Q99257
J	0	SER	-	expression tag	UNP Q99257

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Chain	Residue	Modelled	Actual	Comment	Reference
J	93	ASP	ASN	conflict	UNP Q99257
K	0	SER	-	expression tag	UNP Q99257
K	93	ASP	ASN	conflict	UNP Q99257

- Molecule 2 is a protein called mRNA transport regulator MTR2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	165	Total	C	H	N	O	S	0	0	0
			2597	836	1285	227	240	9			
2	F	164	Total	C	H	N	O	S	0	0	0
			2586	831	1283	225	238	9			
2	I	161	Total	C	H	N	O	S	0	0	0
			2534	816	1256	220	234	8			
2	L	162	Total	C	H	N	O	S	0	0	0
			2551	820	1264	223	236	8			

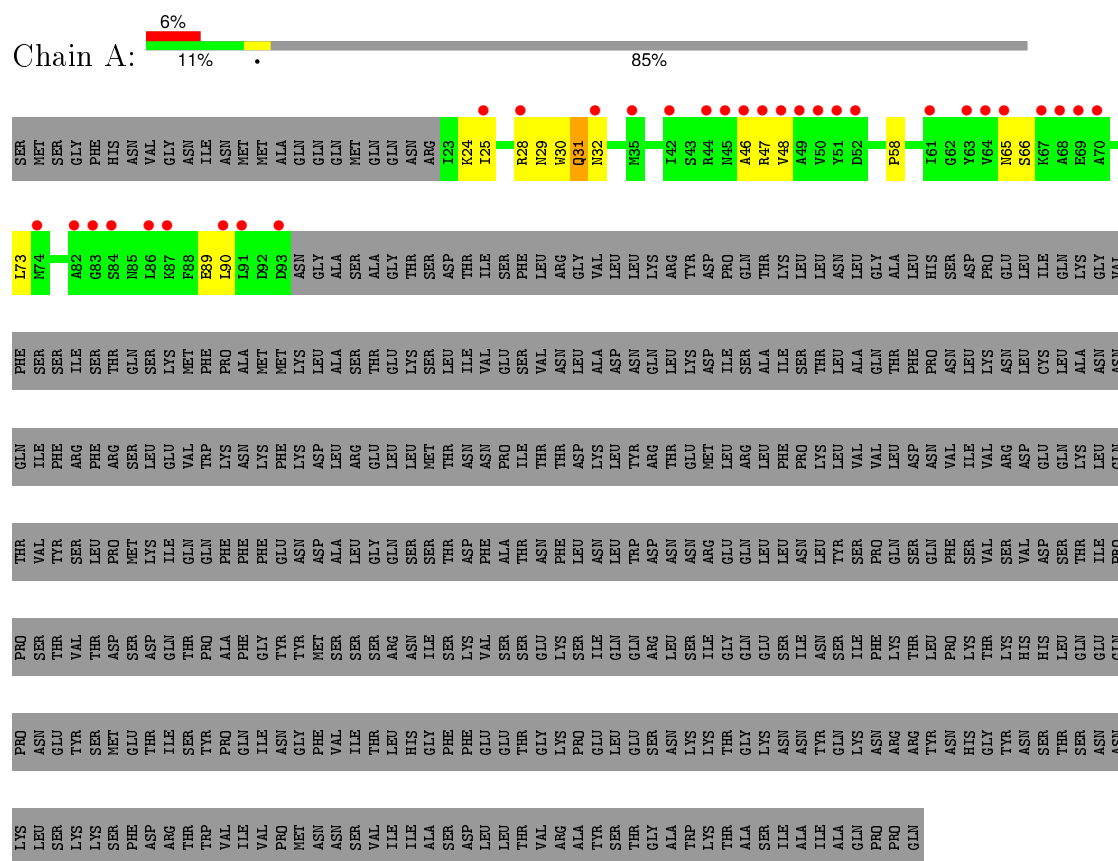
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Zn	0	0
			1	1		
3	J	1	Total	Zn	0	0
			1	1		
3	K	2	Total	Zn	0	0
			2	2		
3	E	2	Total	Zn	0	0
			2	2		
3	H	1	Total	Zn	0	0
			1	1		
3	B	3	Total	Zn	0	0
			3	3		
3	C	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

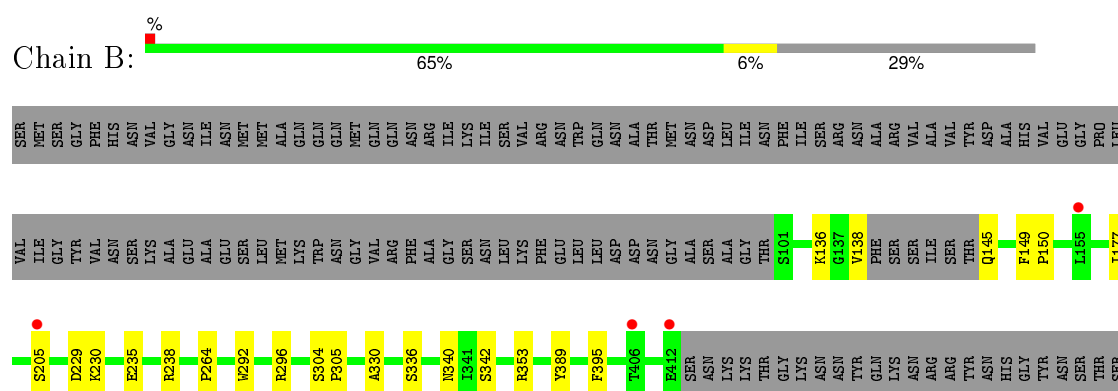
### 3 Residue-property plots

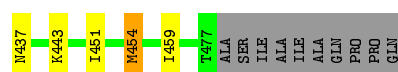
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: mRNA export factor MEX67

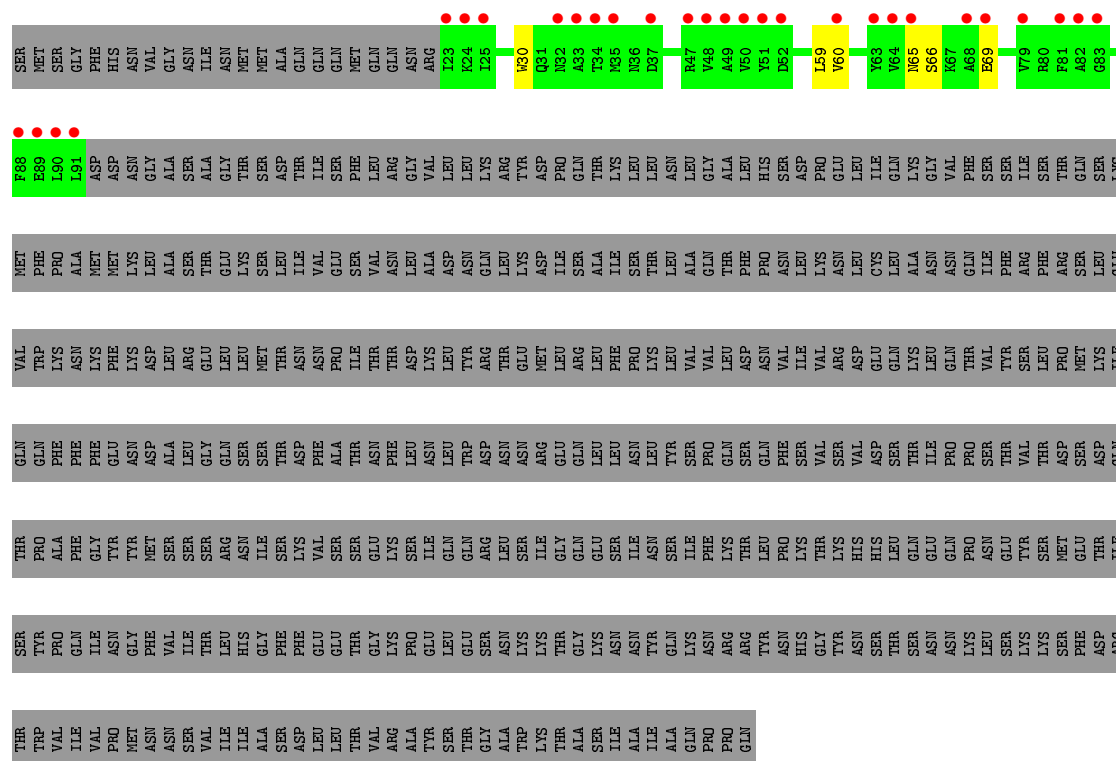


- Molecule 1: mRNA export factor MEX67

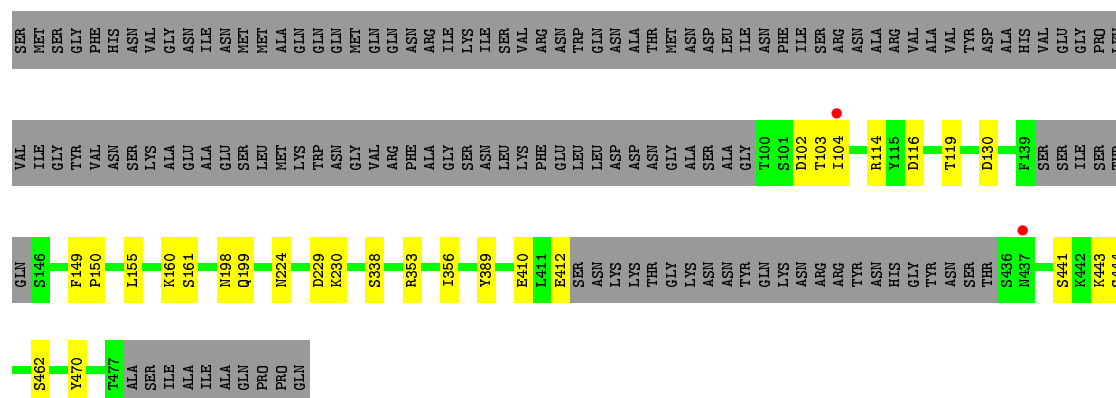




• Molecule 1: mRNA export factor MEX67

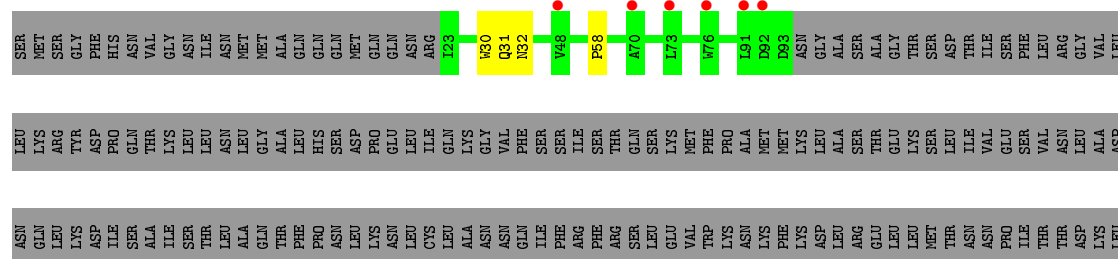


• Molecule 1: mRNA export factor MEX67



• Molecule 1: mRNA export factor MEX67



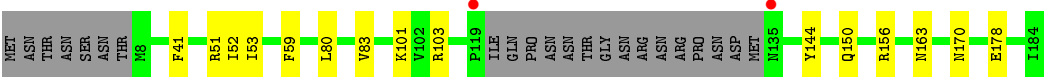
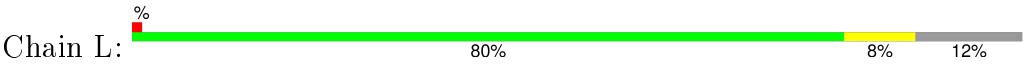








● Molecule 2: mRNA transport regulator MTR2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.61Å 76.72Å 199.12Å 90.00° 94.09° 90.00°	Depositor
Resolution (Å)	49.65 – 3.30 49.65 – 3.30	Depositor EDS
% Data completeness (in resolution range)	86.8 (49.65-3.30) 86.9 (49.65-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.228 , 0.284 0.228 , 0.286	Depositor DCC
$R_{free}$ test set	1988 reflections (4.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.4	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	2 of 40074 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	37509	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	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 35.94 % 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 5.3969e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.28	0/574	0.48	0/776
1	B	0.27	0/2842	0.45	0/3845
1	D	0.27	0/558	0.48	0/754
1	E	0.26	0/2858	0.45	0/3867
1	G	0.26	0/558	0.47	0/754
1	H	0.28	0/2971	0.46	0/4023
1	J	0.25	0/574	0.47	0/776
1	K	0.27	0/2931	0.46	0/3967
2	C	0.27	0/1341	0.45	0/1819
2	F	0.26	0/1332	0.46	0/1807
2	I	0.28	0/1307	0.44	0/1774
2	L	0.28	0/1316	0.47	0/1786
All	All	0.27	0/19162	0.46	0/25948

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	564	555	559	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2789	2805	2810	13	0
1	D	548	551	551	5	0
1	E	2804	2817	2823	15	0
1	G	548	551	551	2	0
1	H	2913	2916	2917	16	1
1	J	564	555	559	2	0
1	K	2875	2874	2879	13	1
2	C	1312	1285	1291	4	0
2	F	1303	1283	1283	7	0
2	I	1278	1256	1256	10	0
2	L	1287	1264	1263	8	0
3	B	3	0	0	0	1
3	C	1	0	0	0	0
3	E	2	0	0	0	1
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	K	2	0	0	0	0
All	All	18797	18712	18742	96	2

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 3.

All (96) 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:E:116:ASP:OD2	1:E:119:THR:HG22	1.59	1.01
1:B:336:SER:O	1:B:353:ARG:NH1	2.06	0.89
2:I:156:ARG:NH2	2:I:163:ASN:O	2.16	0.79
1:B:292:TRP:O	1:B:296:ARG:NH1	2.16	0.78
1:E:116:ASP:OD2	1:E:119:THR:CG2	2.38	0.71
1:A:25:ILE:HD13	1:A:90:LEU:HD21	1.74	0.70
1:K:338:SER:O	1:K:353:ARG:NH1	2.25	0.69
1:D:65:ASN:OD1	1:D:66:SER:N	2.27	0.68
1:K:174:LEU:N	1:K:198:ASN:OD1	2.26	0.68
1:A:31:GLN:O	1:A:32:ASN:ND2	2.28	0.67
2:I:77:GLN:OE1	2:I:103:ARG:NH2	2.28	0.66
1:H:338:SER:O	1:H:353:ARG:NH1	2.28	0.66
2:L:156:ARG:NH2	2:L:163:ASN:O	2.28	0.65
2:F:46:ASN:ND2	2:F:49:ASN:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ASN:OD1	1:A:66:SER:N	2.31	0.64
1:E:116:ASP:CG	1:E:119:THR:HG22	2.19	0.63
1:K:292:TRP:O	1:K:296:ARG:NH1	2.31	0.63
1:H:141:SER:HG	1:H:144:THR:HG1	1.48	0.62
1:E:338:SER:O	1:E:353:ARG:NH1	2.33	0.60
1:H:377:GLU:OE1	1:H:377:GLU:N	2.34	0.60
1:K:149:PHE:HB2	1:K:150:PRO:HD3	1.84	0.59
1:H:433:ASN:ND2	1:H:435:THR:OG1	2.37	0.56
1:H:116:ASP:OD2	1:H:119:THR:HG23	2.05	0.56
1:D:69:GLU:OE2	1:D:69:GLU:N	2.39	0.55
1:E:198:ASN:O	1:E:224:ASN:ND2	2.40	0.55
1:K:273:GLU:OE1	1:K:388:SER:OG	2.25	0.54
1:B:395:PHE:CZ	1:B:451:ILE:HD11	2.42	0.54
1:B:235:GLU:OE2	1:B:238:ARG:NH2	2.33	0.54
1:A:24:LYS:O	1:A:90:LEU:HD23	2.08	0.53
1:B:229:ASP:OD1	1:B:230:LYS:N	2.43	0.51
1:E:229:ASP:OD1	1:E:230:LYS:N	2.43	0.51
1:E:441:SER:OG	1:E:443:LYS:NZ	2.43	0.51
1:K:160:LYS:O	1:K:161:SER:OG	2.21	0.51
1:E:356:ILE:HD13	2:F:9:VAL:HG21	1.92	0.51
1:K:296:ARG:NH2	1:K:369:PRO:O	2.44	0.50
1:H:268:GLN:HB2	2:I:56:ALA:HB3	1.92	0.50
1:E:149:PHE:HB2	1:E:150:PRO:HD3	1.94	0.50
1:A:46:ALA:O	1:A:47:ARG:HG2	2.11	0.50
1:B:138:VAL:HG23	1:B:145:GLN:HG2	1.94	0.49
1:H:364:ILE:O	1:H:367:THR:OG1	2.26	0.48
1:B:177:ILE:N	1:B:205:SER:OG	2.42	0.48
1:B:330:ALA:O	1:B:443:LYS:NZ	2.37	0.47
1:J:30:TRP:NE1	1:J:58:PRO:O	2.45	0.47
1:H:335:MET:HG3	1:H:435:THR:HB	1.96	0.47
1:B:149:PHE:HB2	1:B:150:PRO:HD3	1.97	0.47
2:L:52:ILE:HB	2:L:59:PHE:HB2	1.97	0.47
2:F:138:ARG:NH1	2:I:36:ASN:OD1	2.48	0.47
1:H:395:PHE:CE2	1:H:451:ILE:HD11	2.50	0.47
1:B:340:ASN:OD1	1:B:342:SER:OG	2.23	0.47
1:B:304:SER:HB2	1:B:305:PRO:HD2	1.97	0.46
1:H:160:LYS:O	1:H:161:SER:OG	2.24	0.46
1:J:31:GLN:O	1:J:32:ASN:HB2	2.16	0.46
2:F:156:ARG:NH2	2:F:163:ASN:O	2.50	0.45
2:I:146:GLY:HA3	2:I:175:TYR:CE2	2.51	0.45
2:I:84:ASP:OD1	2:I:85:TYR:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:ARG:HH21	1:E:130:ASP:HB2	1.82	0.44
1:A:25:ILE:HD13	1:A:90:LEU:CD2	2.45	0.44
1:H:229:ASP:OD1	1:H:230:LYS:N	2.51	0.44
1:B:264:PRO:HG3	2:C:72:GLN:HB3	1.99	0.44
1:A:30:TRP:NE1	1:A:58:PRO:O	2.50	0.44
1:K:387:ILE:CG2	2:L:53:ILE:HD11	2.48	0.43
1:E:462:SER:HB2	2:F:86:HIS:HD1	1.83	0.43
2:I:101:LYS:HB3	2:I:144:TYR:CD1	2.53	0.43
1:G:47:ARG:HA	1:G:47:ARG:HD2	1.90	0.43
2:L:103:ARG:HG3	2:L:144:TYR:CE1	2.54	0.43
2:F:101:LYS:HB3	2:F:144:TYR:CD1	2.54	0.43
2:I:102:VAL:HG21	2:I:147:ILE:HD12	2.01	0.43
1:A:48:VAL:HG21	1:A:73:LEU:HB2	2.00	0.43
1:H:274:ASN:OD1	1:H:275:ASP:N	2.52	0.43
1:K:229:ASP:OD1	1:K:230:LYS:N	2.52	0.43
1:H:468:ARG:NH2	2:I:174:VAL:HB	2.34	0.42
1:E:104:ILE:HG23	1:E:155:LEU:HD21	2.01	0.42
2:C:154:ASP:OD2	2:C:156:ARG:NH1	2.52	0.42
1:D:30:TRP:HE1	1:D:59:LEU:HA	1.85	0.42
1:A:28:ARG:HG2	1:A:29:ASN:N	2.35	0.42
1:E:102:ASP:OD1	1:E:103:THR:N	2.53	0.42
2:L:150:GLN:HB2	2:L:170:ASN:HB3	2.01	0.41
1:K:388:SER:O	2:L:51:ARG:NH1	2.53	0.41
2:L:101:LYS:HB3	2:L:144:TYR:CD1	2.54	0.41
1:B:454:MET:HG3	1:B:459:ILE:HD13	2.01	0.41
2:F:80:LEU:O	1:H:255:GLN:NE2	2.46	0.41
1:E:160:LYS:O	1:E:161:SER:OG	2.22	0.41
2:C:105:ASP:OD1	2:C:107:SER:OG	2.24	0.41
1:K:362:ASN:OD1	1:K:366:LYS:NZ	2.53	0.41
1:H:339:ARG:NH1	1:H:350:ILE:O	2.46	0.41
1:H:136:LYS:HD3	1:H:136:LYS:HA	1.98	0.41
1:E:444:SER:HB2	1:E:470:TYR:HA	2.01	0.41
1:K:203:PHE:CE1	1:K:226:ILE:HG21	2.56	0.41
1:K:428:TYR:CG	1:K:429:ASN:N	2.89	0.41
1:A:89:GLU:HG2	1:A:90:LEU:N	2.36	0.41
2:L:80:LEU:HD11	2:L:83:VAL:CG2	2.51	0.40
2:I:147:ILE:HD13	2:I:171:TYR:CE1	2.56	0.40
1:D:30:TRP:NE1	1:D:60:VAL:HG23	2.36	0.40
1:D:30:TRP:CE2	1:D:60:VAL:HG23	2.56	0.40
1:G:28:ARG:HG2	1:G:29:ASN:N	2.37	0.40
2:C:150:GLN:HB2	2:C:170:ASN:HB3	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:374:HIS:HE2	3:B:501:ZN:ZN[1_655]	1.32	0.28
1:H:430:HIS:HE2	3:E:501:ZN:ZN[2_647]	1.54	0.06

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	69/488 (14%)	65 (94%)	4 (6%)	0	100	100
1	B	341/488 (70%)	336 (98%)	5 (2%)	0	100	100
1	D	67/488 (14%)	63 (94%)	4 (6%)	0	100	100
1	E	343/488 (70%)	341 (99%)	2 (1%)	0	100	100
1	G	67/488 (14%)	62 (92%)	5 (8%)	0	100	100
1	H	359/488 (74%)	351 (98%)	8 (2%)	0	100	100
1	J	69/488 (14%)	63 (91%)	6 (9%)	0	100	100
1	K	352/488 (72%)	347 (99%)	5 (1%)	0	100	100
2	C	161/184 (88%)	159 (99%)	2 (1%)	0	100	100
2	F	160/184 (87%)	160 (100%)	0	0	100	100
2	I	157/184 (85%)	156 (99%)	1 (1%)	0	100	100
2	L	158/184 (86%)	157 (99%)	1 (1%)	0	100	100
All	All	2303/4640 (50%)	2260 (98%)	43 (2%)	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	60/442 (14%)	59 (98%)	1 (2%)	68	86
1	B	324/442 (73%)	320 (99%)	4 (1%)	78	90
1	D	58/442 (13%)	58 (100%)	0	100	100
1	E	326/442 (74%)	322 (99%)	4 (1%)	78	90
1	G	58/442 (13%)	57 (98%)	1 (2%)	68	86
1	H	339/442 (77%)	333 (98%)	6 (2%)	66	85
1	J	60/442 (14%)	60 (100%)	0	100	100
1	K	334/442 (76%)	330 (99%)	4 (1%)	78	90
2	C	145/163 (89%)	144 (99%)	1 (1%)	88	94
2	F	144/163 (88%)	143 (99%)	1 (1%)	88	94
2	I	141/163 (86%)	138 (98%)	3 (2%)	61	84
2	L	142/163 (87%)	140 (99%)	2 (1%)	74	88
All	All	2131/4188 (51%)	2104 (99%)	27 (1%)	76	89

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	B	136	LYS
1	B	389	TYR
1	B	437	ASN
1	B	454	MET
2	C	10	MET
1	E	199	GLN
1	E	389	TYR
1	E	410	GLU
1	E	412	GLU
2	F	41	PHE
1	G	54	HIS
1	H	136	LYS
1	H	176	ASP
1	H	389	TYR
1	H	412	GLU
1	H	462	SER
1	H	468	ARG

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Mol	Chain	Res	Type
2	I	41	PHE
2	I	94	LEU
2	I	178	GLU
1	K	248	ASN
1	K	389	TYR
1	K	411	LEU
1	K	462	SER
2	L	41	PHE
2	L	178	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	71/488 (14%)	1.93	31 (43%) 0 0	91, 113, 136, 146	0
1	B	347/488 (71%)	0.17	4 (1%) 81 76	22, 52, 85, 110	0
1	D	69/488 (14%)	2.06	28 (40%) 0 0	93, 114, 140, 165	0
1	E	349/488 (71%)	0.26	2 (0%) 90 88	27, 56, 88, 103	0
1	G	69/488 (14%)	0.54	1 (1%) 78 73	49, 73, 92, 96	0
1	H	363/488 (74%)	0.28	16 (4%) 38 31	20, 50, 93, 124	0
1	J	71/488 (14%)	0.73	6 (8%) 13 10	41, 74, 99, 106	0
1	K	358/488 (73%)	0.18	12 (3%) 49 42	16, 42, 88, 112	0
2	C	165/184 (89%)	-0.07	1 (0%) 90 88	19, 36, 69, 96	0
2	F	164/184 (89%)	-0.04	1 (0%) 90 88	26, 42, 73, 92	0
2	I	161/184 (87%)	-0.10	3 (1%) 70 63	17, 37, 69, 98	0
2	L	162/184 (88%)	-0.11	2 (1%) 81 76	19, 31, 62, 107	0
All	All	2349/4640 (50%)	0.27	107 (4%) 36 30	16, 50, 107, 165	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	51	TYR	8.4
1	A	50	VAL	6.9
1	A	48	VAL	6.3
1	K	118	GLN	5.4
1	H	143	SER	5.3
1	D	65	ASN	5.2
1	A	46	ALA	5.0
1	D	52	ASP	4.7
2	L	135	ASN	4.5
1	K	176	ASP	4.4
1	D	50	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	69	GLU	4.3
1	K	202	ARG	4.1
1	A	49	ALA	4.1
1	D	49	ALA	4.0
1	A	25	ILE	4.0
1	D	90	LEU	3.9
2	I	120	ILE	3.9
1	H	345	SER	3.9
1	D	33	ALA	3.8
1	K	222	THR	3.7
1	D	24	LYS	3.6
1	D	64	VAL	3.4
1	D	23	ILE	3.4
1	A	83	GLY	3.3
2	F	8	MET	3.2
1	D	32	ASN	3.2
1	A	42	ILE	3.2
1	A	52	ASP	3.2
1	H	139	PHE	3.2
1	D	35	MET	3.2
1	A	63	TYR	3.2
1	H	231	LEU	3.1
1	A	70	ALA	3.1
1	D	69	GLU	3.0
1	D	89	GLU	3.0
1	D	91	LEU	3.0
2	I	119	PRO	2.9
1	K	145	GLN	2.9
1	A	51	TYR	2.9
1	D	63	TYR	2.9
1	D	68	ALA	2.8
1	J	92	ASP	2.8
1	D	47	ARG	2.8
1	B	155	LEU	2.8
1	H	140	SER	2.8
1	J	73	LEU	2.8
1	H	118	GLN	2.8
1	A	44	ARG	2.8
1	H	141	SER	2.7
1	D	25	ILE	2.7
1	A	87	LYS	2.7
1	H	230	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	45	ASN	2.7
1	A	61	ILE	2.6
1	J	48	VAL	2.6
1	H	433	ASN	2.6
1	J	91	LEU	2.6
2	C	120	ILE	2.6
1	K	345	SER	2.6
2	L	119	PRO	2.6
1	D	34	THR	2.6
1	D	79	VAL	2.5
1	D	37	ASP	2.5
1	H	203	PHE	2.5
1	K	111	LEU	2.5
1	A	68	ALA	2.5
1	A	64	VAL	2.4
1	A	86	LEU	2.4
1	H	176	ASP	2.4
1	A	28	ARG	2.4
1	D	81	PHE	2.4
1	A	74	MET	2.4
1	A	65	ASN	2.4
1	D	60	VAL	2.4
1	A	67	LYS	2.3
1	A	32	ASN	2.3
1	H	428	TYR	2.3
1	D	83	GLY	2.3
1	K	228	THR	2.3
1	H	202	ARG	2.3
1	J	70	ALA	2.2
1	D	48	VAL	2.2
1	H	435	THR	2.2
1	D	82	ALA	2.2
1	A	82	ALA	2.2
1	K	206	LEU	2.2
1	A	84	SER	2.2
1	E	104	ILE	2.2
1	H	145	GLN	2.2
2	I	114	GLN	2.2
1	K	112	LEU	2.2
1	A	47	ARG	2.2
1	D	88	PHE	2.2
1	A	93	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	203	PHE	2.1
1	B	412	GLU	2.1
1	A	35	MET	2.1
1	J	76	TRP	2.1
1	B	205	SER	2.1
1	B	406	THR	2.1
1	K	180	ILE	2.1
1	E	437	ASN	2.0
1	A	90	LEU	2.0
1	H	124	LEU	2.0
1	G	65	ASN	2.0
1	A	91	LEU	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	F	201	1/1	0.99	0.20	0.28	10,10,10,10	0
3	ZN	E	501	1/1	0.91	0.26	0.00	108,108,108,108	0
3	ZN	C	201	1/1	0.98	0.17	-1.14	22,22,22,22	0
3	ZN	B	503	1/1	0.96	0.12	-1.53	60,60,60,60	0
3	ZN	J	501	1/1	0.91	0.08	-2.12	80,80,80,80	0
3	ZN	E	502	1/1	0.97	0.13	-2.14	37,37,37,37	0
3	ZN	B	502	1/1	0.96	0.10	-2.26	51,51,51,51	0
3	ZN	K	502	1/1	0.96	0.11	-2.70	59,59,59,59	0
3	ZN	B	501	1/1	0.99	0.10	-4.11	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	G	501	1/1	0.99	0.05	-	81,81,81,81	0
3	ZN	H	501	1/1	0.97	0.15	-	54,54,54,54	0
3	ZN	K	501	1/1	0.96	0.13	-	47,47,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.