



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:03 am BST

PDB ID : 4R8P
Title : Crystal structure of the Ring1B/Bmi1/UbcH5c PRC1 ubiquitylation module bound to the nucleosome core particle
Authors : McGinty, R.K.; Henrici, R.C.; Tan, S.
Deposited on : 2014-09-02
Resolution : 3.28 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

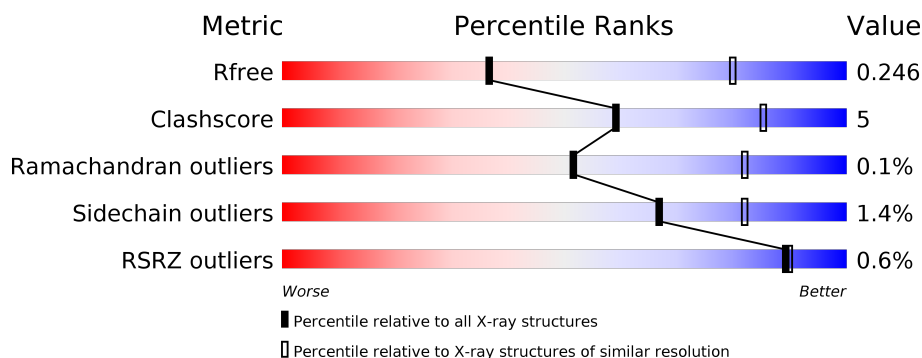
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.28 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}	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	135	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 67%; background-color: green;"></div> <div style="width: 6%; background-color: yellow;"></div> <div style="width: 27%; background-color: grey;"></div> </div> </div> </div>
1	E	135	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 66%; background-color: green;"></div> <div style="width: 6%; background-color: yellow;"></div> <div style="width: 28%; background-color: grey;"></div> </div> </div> </div>
2	B	102	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 76%; background-color: green;"></div> <div style="width: 8%; background-color: yellow;"></div> <div style="width: 16%; background-color: grey;"></div> </div> </div> </div>
2	F	102	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 73%; background-color: green;"></div> <div style="width: 8%; background-color: yellow;"></div> <div style="width: 20%; background-color: grey;"></div> </div> </div> </div>
3	C	129	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 67%; background-color: green;"></div> <div style="width: 14%; background-color: yellow;"></div> <div style="width: 19%; background-color: grey;"></div> </div> </div> </div>
3	G	129	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 77%; background-color: green;"></div> <div style="width: 6%; background-color: yellow;"></div> <div style="width: 17%; background-color: grey;"></div> </div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	122	<div><div></div><div>71%7%22%</div></div>
4	H	122	<div><div></div><div>72%6%22%</div></div>
5	I	147	<div><div></div><div>76%22%•</div></div>
6	J	147	<div><div></div><div>%75%24%•</div></div>
7	K	110	<div><div></div><div>3%83%13%5%</div></div>
7	M	110	<div><div></div><div>75%13%12%</div></div>
8	L	268	<div><div></div><div>%74%19%• 5%</div></div>
8	N	268	<div><div></div><div>81%13%6%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 17134 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 Histone H3.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			789	500	147	139	3			
1	E	97	Total	C	N	O	S	0	0	0
			788	498	151	136	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	CONFLICT	UNP P84233
E	102	ALA	GLY	CONFLICT	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	86	Total	C	N	O	S	0	0	0
			675	424	133	117	1			
2	F	82	Total	C	N	O	S	0	0	0
			635	400	121	113	1			

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	104	Total	C	N	O		0	0	0
			766	483	143	140				
3	G	107	Total	C	N	O		0	0	0
			793	498	152	143				

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	95	Total	C	N	O	S	0	0	0
			721	453	127	139	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	95	Total	C	N	O	S	0	0	0
			719	451	126	140	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	32	THR	SER	CONFLICT	UNP P02281
H	32	THR	SER	CONFLICT	UNP P02281

- Molecule 5 is a DNA chain called DNA (147-mer).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	144	Total	C	N	O	P	0	0	0
			2935	1393	536	862	144			

- Molecule 6 is a DNA chain called DNA (147-mer).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	145	Total	C	N	O	P	0	0	0
			2990	1415	559	871	145			

- Molecule 7 is a protein called Polycomb complex protein BMI-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	K	105	Total	C	N	O	S	0	0	0
			819	523	141	146	9			
7	M	97	Total	C	N	O	S	0	0	0
			744	477	128	131	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	0	GLY	-	EXPRESSION TAG	UNP P35226
K	1	SER	-	EXPRESSION TAG	UNP P35226
M	0	GLY	-	EXPRESSION TAG	UNP P35226
M	1	SER	-	EXPRESSION TAG	UNP P35226

- Molecule 8 is a protein called E3 ubiquitin-protein ligase RING2, Ubiquitin-conjugating enzyme E2 D3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	L	254	Total	C	N	O	S	0	0	0
			1857	1179	315	348	15			
8	N	253	Total	C	N	O	S	0	0	0
			1895	1205	321	353	16			

There are 14 discrepancies between the modelled and reference sequences:

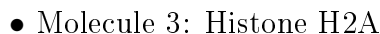
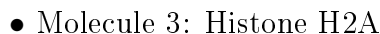
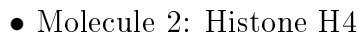
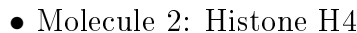
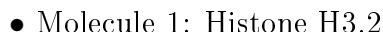
Chain	Residue	Modelled	Actual	Comment	Reference
L	1	GLY	-	EXPRESSION TAG	UNP Q99496
L	117	GLY	-	LINKER	UNP Q99496
L	118	SER	-	LINKER	UNP Q99496
L	119	GLY	-	LINKER	UNP Q99496
L	120	SER	-	LINKER	UNP Q99496
L	121	ARG	-	LINKER	UNP Q99496
L	122	SER	-	LINKER	UNP Q99496
N	1	GLY	-	EXPRESSION TAG	UNP Q99496
N	117	GLY	-	LINKER	UNP Q99496
N	118	SER	-	LINKER	UNP Q99496
N	119	GLY	-	LINKER	UNP Q99496
N	120	SER	-	LINKER	UNP Q99496
N	121	ARG	-	LINKER	UNP Q99496
N	122	SER	-	LINKER	UNP Q99496

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	2	Total	Zn	0	0
			2	2		
9	K	2	Total	Zn	0	0
			2	2		
9	N	2	Total	Zn	0	0
			2	2		
9	M	2	Total	Zn	0	0
			2	2		

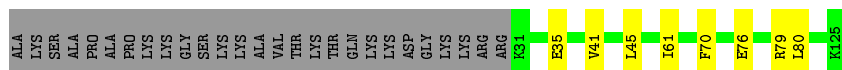
i

- Molecule 1: Histone H3.2

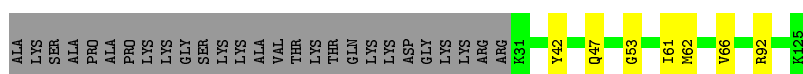




- Molecule 4: Histone H2B 1.1



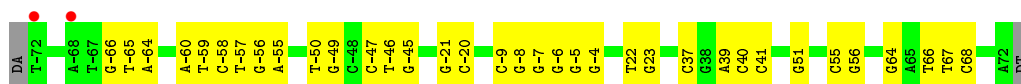
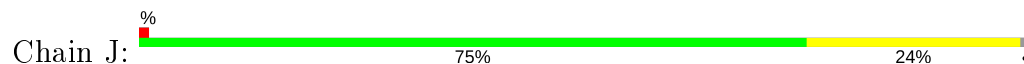
- Molecule 4: Histone H2B 1.1



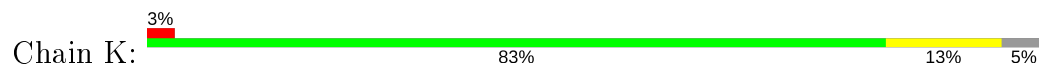
- Molecule 5: DNA (147-mer)



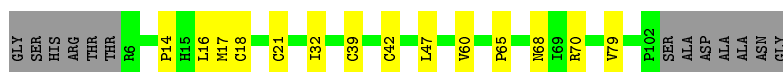
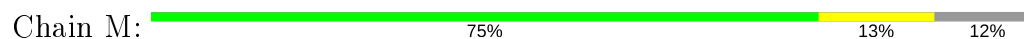
- Molecule 6: DNA (147-mer)



- Molecule 7: Polycomb complex protein BMI-1

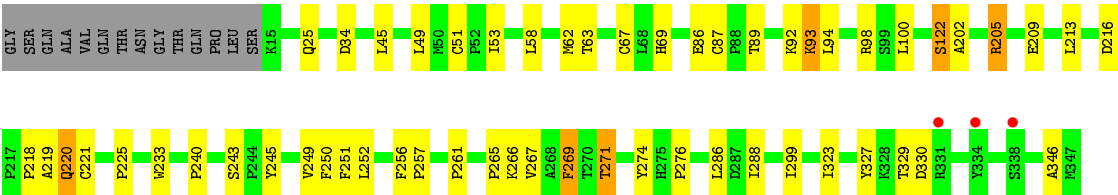


- Molecule 7: Polycomb complex protein BMI-1

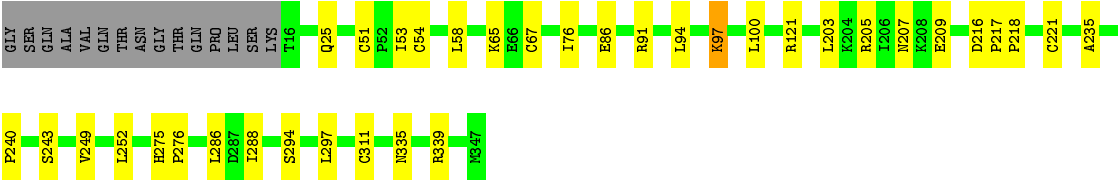
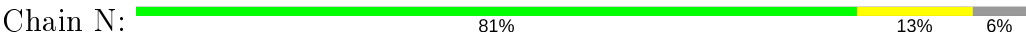


- Molecule 8: E3 ubiquitin-protein ligase RING2, Ubiquitin-conjugating enzyme E2 D3





● Molecule 8: E3 ubiquitin-protein ligase RING2, Ubiquitin-conjugating enzyme E2 D3



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	104.92Å 180.05Å 375.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 3.28 45.00 – 3.28	Depositor EDS
% Data completeness (in resolution range)	99.1 (45.00-3.28) 99.1 (45.00-3.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.197 , 0.245 0.199 , 0.246	Depositor DCC
R_{free} test set	2751 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	105.6	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 77.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.027 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.034 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17134	wwPDB-VP
Average B, all atoms (Å ²)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [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	0.21	0/801	0.37	0/1079
1	E	0.20	0/800	0.35	0/1076
2	B	0.20	0/682	0.38	0/914
2	F	0.20	0/642	0.38	0/864
3	C	0.19	0/776	0.35	0/1058
3	G	0.19	0/803	0.35	0/1093
4	D	0.20	0/732	0.36	0/989
4	H	0.20	0/730	0.36	0/988
5	I	0.46	0/3289	0.85	0/5069
6	J	0.46	0/3357	0.85	0/5184
7	K	0.21	0/836	0.38	0/1136
7	M	0.20	0/761	0.38	0/1038
8	L	0.20	0/1905	0.38	0/2606
8	N	0.20	0/1945	0.37	0/2660
All	All	0.32	0/18059	0.61	0/25754

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	789	0	809	6	0
1	E	788	0	815	7	0
2	B	675	0	704	5	0
2	F	635	0	652	6	0
3	C	766	0	771	13	0
3	G	793	0	805	7	0
4	D	721	0	713	8	0
4	H	719	0	707	5	0
5	I	2935	0	1615	24	0
6	J	2990	0	1628	27	0
7	K	819	0	807	8	0
7	M	744	0	705	8	0
8	L	1857	0	1734	34	0
8	N	1895	0	1804	21	0
9	K	2	0	0	0	0
9	L	2	0	0	0	0
9	M	2	0	0	0	0
9	N	2	0	0	0	0
All	All	17134	0	14269	142	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 (142) 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)
8:L:219:ALA:C	8:L:220:GLN:HG3	1.97	0.85
8:L:219:ALA:O	8:L:220:GLN:HG3	1.80	0.81
5:I:41:DG:H1	6:J:41:DC:H42	1.40	0.70
8:L:53:ILE:O	8:L:205:ARG:NH1	2.26	0.67
8:L:329:THR:N	8:L:330:ASP:HA	2.11	0.64
8:L:218:PRO:HG2	8:L:221:CYS:HB2	1.80	0.62
7:M:16:LEU:HD22	7:M:79:VAL:HG22	1.82	0.62
8:N:205:ARG:NH1	8:N:209:GLU:OE2	2.33	0.61
7:M:32:ILE:HD11	7:M:70:ARG:HH11	1.67	0.60
1:A:108:ASN:ND2	2:B:42:GLY:O	2.36	0.59
8:N:294:SER:HB3	8:N:297:LEU:HG	1.83	0.59
1:A:49:ARG:NH2	6:J:65:DT:OP1	2.35	0.58
7:M:60:VAL:O	7:M:68:ASN:ND2	2.36	0.58
3:C:102:ILE:HG23	4:D:61:ILE:HD13	1.85	0.58
7:M:47:LEU:HD13	7:M:65:PRO:HB2	1.84	0.58
6:J:68:DC:OP1	8:L:266:LYS:NZ	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ILE:HD12	1:E:130:ILE:HD12	1.87	0.57
7:K:16:LEU:HD22	7:K:79:VAL:HG12	1.86	0.57
3:G:42:ARG:HG2	5:I:39:DA:H5'	1.87	0.57
3:C:32:ARG:NH2	4:D:35:GLU:OE2	2.33	0.57
7:M:39:CYS:HB2	7:M:42:CYS:SG	2.43	0.56
5:I:-64:DC:H42	6:J:64:DG:H1	1.54	0.56
8:L:62:MET:HB3	8:L:100:LEU:HD13	1.86	0.56
8:L:276:PRO:HD3	8:L:323:ILE:HG21	1.88	0.56
2:B:60:VAL:O	2:B:64:ASN:ND2	2.39	0.56
5:I:7:DC:H42	6:J:-7:DG:H1	1.55	0.55
5:I:4:DC:H42	6:J:-4:DG:H1	1.55	0.55
6:J:-21:DG:H2"	6:J:-20:DC:H5"	1.90	0.54
8:N:65:LYS:NZ	8:N:100:LEU:O	2.41	0.54
8:N:235:ALA:HB3	8:N:252:LEU:HB2	1.89	0.54
3:C:30:VAL:HG13	4:D:70:PHE:HE1	1.73	0.54
3:C:112:GLN:HB2	3:C:115:LEU:HD13	1.89	0.54
8:L:86:GLU:HA	8:L:93:LYS:HA	1.90	0.53
3:G:24:GLN:NE2	4:H:47:GLN:OE1	2.41	0.53
8:N:243:SER:HB2	8:N:311:CYS:HA	1.90	0.53
7:K:60:VAL:O	7:K:68:ASN:ND2	2.42	0.53
3:G:76:THR:O	4:H:53:GLY:N	2.39	0.52
8:N:218:PRO:HB2	8:N:221:CYS:HB2	1.90	0.52
7:K:82:LEU:HD21	8:L:45:LEU:HD11	1.92	0.52
1:E:44:GLY:O	2:F:44:LYS:NZ	2.43	0.52
6:J:-60:DA:H2"	6:J:-59:DT:H5'	1.91	0.52
8:N:249:VAL:O	8:N:249:VAL:HG12	2.10	0.52
7:K:47:LEU:HD13	7:K:65:PRO:HB2	1.92	0.51
8:L:251:PHE:H	8:L:271:THR:HG21	1.75	0.51
3:C:92:GLU:OE1	8:L:98:ARG:NH1	2.43	0.51
3:C:113:SER:HA	3:C:116:LEU:HD23	1.93	0.50
1:E:63:ARG:HE	5:I:17:DA:H4'	1.76	0.50
5:I:20:DG:H2"	5:I:21:DC:H5'	1.93	0.50
8:L:252:LEU:HD13	8:L:267:VAL:HG13	1.92	0.50
5:I:-51:DC:H42	6:J:51:DG:H1	1.60	0.50
8:N:240:PRO:HG2	8:N:243:SER:HB3	1.92	0.50
2:F:47:SER:HB3	2:F:50:ILE:HG12	1.94	0.49
1:A:60:LEU:HD12	1:A:64:LYS:HE3	1.93	0.49
8:L:205:ARG:HH11	8:L:261:PRO:HG3	1.77	0.49
1:E:43:PRO:HA	5:I:9:DG:H5'	1.95	0.49
8:L:216:ASP:N	8:L:216:ASP:OD1	2.45	0.49
8:L:225:PRO:HA	8:L:233:TRP:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:75:HIS:O	4:H:92:ARG:NH1	2.33	0.49
3:C:63:LEU:HD13	4:D:45:LEU:HB2	1.94	0.48
8:L:329:THR:OG1	8:L:330:ASP:O	2.31	0.48
7:M:18:CYS:HB3	7:M:21:CYS:SG	2.52	0.48
3:G:90:ASP:HB3	3:G:93:LEU:HB2	1.96	0.48
7:K:12:LEU:HD23	7:K:82:LEU:HD13	1.95	0.48
3:G:42:ARG:HE	5:I:38:DT:H4'	1.79	0.48
5:I:15:DT:H2''	5:I:16:DA:C8	2.49	0.47
8:N:203:LEU:O	8:N:207:ASN:ND2	2.45	0.47
8:N:54:CYS:SG	8:N:121:ARG:NH1	2.87	0.47
8:N:51:CYS:HB2	8:N:58:LEU:HD23	1.96	0.47
3:C:63:LEU:HD11	4:D:41:VAL:HG13	1.96	0.47
3:C:80:PRO:HB3	4:D:61:ILE:HD12	1.96	0.47
8:L:245:TYR:OH	8:L:274:TYR:O	2.29	0.47
3:C:69:ALA:O	3:C:73:ASN:ND2	2.38	0.47
2:B:35:ARG:O	2:B:39:ARG:HG2	2.14	0.47
5:I:-59:DT:H2''	5:I:-58:DG:C8	2.50	0.47
8:N:216:ASP:OD1	8:N:216:ASP:N	2.48	0.47
6:J:-57:DT:H2''	6:J:-56:DG:C8	2.50	0.46
1:E:119:ILE:HD11	2:F:46:ILE:HG23	1.97	0.46
3:G:79:ILE:HG12	3:G:82:HIS:CE1	2.51	0.46
5:I:58:DG:H1	6:J:-58:DC:H42	1.63	0.46
7:K:31:ILE:HG22	7:K:69:ILE:HG22	1.97	0.46
5:I:-37:DG:H1	6:J:37:DC:H5	1.63	0.46
8:N:217:PRO:HA	8:N:218:PRO:HD3	1.85	0.46
3:C:90:ASP:HB3	3:C:93:LEU:HB2	1.98	0.46
8:L:45:LEU:HB3	8:L:49:LEU:HD13	1.97	0.46
3:G:102:ILE:HG23	4:H:61:ILE:HD13	1.99	0.45
5:I:57:DA:H61	6:J:-57:DT:H3	1.65	0.45
8:L:51:CYS:HB2	8:L:58:LEU:HD23	1.98	0.45
1:A:73:GLU:O	1:A:76:GLN:HG2	2.17	0.45
6:J:-50:DT:H2''	6:J:-49:DG:C8	2.52	0.45
8:L:220:GLN:HB2	8:L:220:GLN:HE21	1.58	0.45
8:N:53:ILE:O	8:N:205:ARG:NE	2.34	0.45
6:J:39:DA:H2''	6:J:40:DC:H5'	1.97	0.45
5:I:-48:DC:H2''	5:I:-47:DT:C5	2.50	0.45
8:L:219:ALA:O	8:L:220:GLN:CG	2.60	0.45
8:L:240:PRO:O	8:L:243:SER:OG	2.30	0.45
8:L:122:SER:HA	8:L:202:ALA:HA	1.67	0.45
4:D:76:GLU:OE1	4:D:79:ARG:NH2	2.44	0.44
5:I:-55:DG:N2	6:J:55:DC:O2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:76:ILE:HG12	8:N:100:LEU:HD21	1.98	0.44
8:L:286:LEU:HG	8:L:288:ILE:HG12	2.00	0.44
6:J:-47:DC:H2"	6:J:-46:DT:C5	2.53	0.44
8:N:86:GLU:HB3	8:N:91:ARG:HA	1.98	0.44
8:N:94:LEU:HD21	8:N:100:LEU:HD11	1.99	0.44
8:L:87:CYS:N	8:L:92:LYS:O	2.44	0.43
7:M:14:PRO:HA	7:M:17:MET:HB2	1.99	0.43
1:E:61:LEU:HG	2:F:36:ARG:HB3	2.01	0.43
2:F:24:ASP:OD1	2:F:25:ASN:N	2.44	0.43
5:I:-69:DA:H2"	5:I:-68:DG:H5'	2.00	0.43
3:C:17:ARG:NH2	3:C:28:GLY:HA2	2.34	0.43
6:J:-9:DC:H2"	6:J:-8:DG:C8	2.54	0.42
6:J:-46:DT:H2"	6:J:-45:DG:C8	2.55	0.42
7:K:35:LEU:HD11	8:L:63:THR:HB	2.01	0.42
8:L:69:HIS:ND1	8:L:89:THR:OG1	2.50	0.42
5:I:-67:DA:H61	6:J:67:DT:H3	1.67	0.42
8:N:286:LEU:HG	8:N:288:ILE:HG12	2.01	0.42
6:J:-6:DG:H2"	6:J:-5:DG:C8	2.55	0.42
4:H:62:MET:O	4:H:66:VAL:HG23	2.19	0.42
8:N:335:ASN:HB3	8:N:339:ARG:NH1	2.35	0.42
5:I:-62:DC:H2"	5:I:-61:DG:C8	2.55	0.42
8:L:257:PRO:HD3	8:L:265:PRO:HA	2.01	0.42
2:B:47:SER:HB3	2:B:50:ILE:HG12	2.01	0.42
5:I:61:DA:H2"	5:I:62:DT:C5	2.55	0.41
6:J:66:DT:H2"	6:J:67:DT:C5	2.55	0.41
8:L:209:GLU:OE2	8:L:299:ILE:N	2.36	0.41
7:M:32:ILE:HD12	7:M:68:ASN:HA	2.02	0.41
2:B:75:HIS:CD2	4:D:80:LEU:HD22	2.55	0.41
8:L:256:PHE:HA	8:L:257:PRO:HD3	1.89	0.41
8:L:34:ASP:N	8:L:34:ASP:OD1	2.47	0.41
5:I:66:DC:N3	6:J:-66:DG:N2	2.65	0.41
6:J:55:DC:H2"	6:J:56:DG:C8	2.56	0.41
5:I:35:DC:H2"	5:I:36:DC:C5	2.56	0.41
8:L:250:PHE:HB3	8:L:269:PHE:HE1	1.85	0.41
8:N:97:LYS:HE2	8:N:97:LYS:HB2	1.86	0.41
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.55	0.41
6:J:22:DT:H2"	6:J:23:DG:C8	2.56	0.41
8:N:275:HIS:CG	8:N:276:PRO:HD2	2.56	0.40
6:J:-65:DT:H2"	6:J:-64:DA:C8	2.56	0.40
5:I:58:DG:H2"	5:I:59:DA:C8	2.57	0.40
8:L:249:VAL:H	8:L:346:ALA:HB1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:HIS:CG	1:E:126:LEU:HD22	2.57	0.40
6:J:-56:DG:H2"	6:J:-55:DA:N7	2.36	0.40
7:K:38:PHE:HB2	7:K:43:ILE:HB	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	96/135 (71%)	92 (96%)	4 (4%)	0	100	100
1	E	95/135 (70%)	91 (96%)	4 (4%)	0	100	100
2	B	84/102 (82%)	81 (96%)	3 (4%)	0	100	100
2	F	80/102 (78%)	75 (94%)	5 (6%)	0	100	100
3	C	102/129 (79%)	99 (97%)	3 (3%)	0	100	100
3	G	105/129 (81%)	102 (97%)	3 (3%)	0	100	100
4	D	93/122 (76%)	86 (92%)	7 (8%)	0	100	100
4	H	93/122 (76%)	90 (97%)	3 (3%)	0	100	100
7	K	103/110 (94%)	96 (93%)	7 (7%)	0	100	100
7	M	95/110 (86%)	88 (93%)	7 (7%)	0	100	100
8	L	252/268 (94%)	228 (90%)	23 (9%)	1 (0%)	34	67
8	N	251/268 (94%)	232 (92%)	19 (8%)	0	100	100
All	All	1449/1732 (84%)	1360 (94%)	88 (6%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	L	122	SER

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	82/110 (74%)	82 (100%)	0	100	100
1	E	82/110 (74%)	81 (99%)	1 (1%)	71	83
2	B	67/78 (86%)	67 (100%)	0	100	100
2	F	63/78 (81%)	63 (100%)	0	100	100
3	C	75/101 (74%)	75 (100%)	0	100	100
3	G	77/101 (76%)	77 (100%)	0	100	100
4	D	75/102 (74%)	75 (100%)	0	100	100
4	H	75/102 (74%)	74 (99%)	1 (1%)	69	82
7	K	90/99 (91%)	89 (99%)	1 (1%)	73	85
7	M	79/99 (80%)	79 (100%)	0	100	100
8	L	193/242 (80%)	183 (95%)	10 (5%)	23	54
8	N	204/242 (84%)	201 (98%)	3 (2%)	65	81
All	All	1162/1464 (79%)	1146 (99%)	16 (1%)	67	82

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	39	HIS
4	H	42	TYR
7	K	80	TYR
8	L	25	GLN
8	L	67	CYS
8	L	93	LYS
8	L	94	LEU
8	L	205	ARG
8	L	213	LEU
8	L	220	GLN
8	L	269	PHE
8	L	271	THR
8	L	327	TYR
8	N	25	GLN

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Mol	Chain	Res	Type
8	N	67	CYS
8	N	97	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
8	L	25	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](#)

Of 8 ligands modelled in this entry, 8 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 [i](#)

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, 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	98/135 (72%)	-0.16	1 (1%) 82 82	60, 88, 149, 211	0
1	E	97/135 (71%)	-0.20	1 (1%) 82 82	66, 100, 155, 225	0
2	B	86/102 (84%)	-0.29	0 100 100	57, 81, 138, 207	0
2	F	82/102 (80%)	-0.13	0 100 100	66, 93, 136, 171	0
3	C	104/129 (80%)	-0.26	0 100 100	58, 96, 131, 167	0
3	G	107/129 (82%)	-0.21	1 (0%) 84 84	56, 87, 132, 207	0
4	D	95/122 (77%)	-0.29	0 100 100	59, 94, 148, 194	0
4	H	95/122 (77%)	-0.19	0 100 100	63, 93, 133, 169	0
5	I	144/147 (97%)	-0.30	0 100 100	111, 178, 240, 264	0
6	J	145/147 (98%)	-0.21	2 (1%) 75 74	101, 178, 258, 299	0
7	K	105/110 (95%)	-0.14	3 (2%) 51 50	66, 91, 185, 218	0
7	M	97/110 (88%)	-0.23	0 100 100	89, 126, 200, 251	0
8	L	254/268 (94%)	-0.20	3 (1%) 79 78	60, 124, 231, 286	0
8	N	253/268 (94%)	-0.21	0 100 100	78, 139, 202, 237	0
All	All	1762/2026 (86%)	-0.21	11 (0%) 89 90	56, 114, 216, 299	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	L	331	ARG	4.2
1	A	39	HIS	3.5
6	J	-72	DT	2.9
7	K	104	ALA	2.3
3	G	115	LEU	2.2
8	L	334	TYR	2.2
7	K	105	ASP	2.2
1	E	38	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
7	K	4	THR	2.1
6	J	-68	DA	2.1
8	L	338	SER	2.1

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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
9	ZN	M	201	1/1	0.94	0.14	133,133,133,133	0
9	ZN	N	401	1/1	0.99	0.17	93,93,93,93	0
9	ZN	L	401	1/1	0.99	0.17	88,88,88,88	0
9	ZN	N	402	1/1	0.99	0.17	78,78,78,78	0
9	ZN	K	202	1/1	0.99	0.15	66,66,66,66	0
9	ZN	M	202	1/1	0.99	0.14	114,114,114,114	0
9	ZN	K	201	1/1	0.99	0.20	81,81,81,81	0
9	ZN	L	402	1/1	1.00	0.13	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.