



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:32 am GMT

PDB ID : 4W9M  
Title : AMPPNP bound Rad50 in complex with dsDNA  
Authors : Rojowska, A.; Lammens, K.  
Deposited on : 2014-08-27  
Resolution : 2.70 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

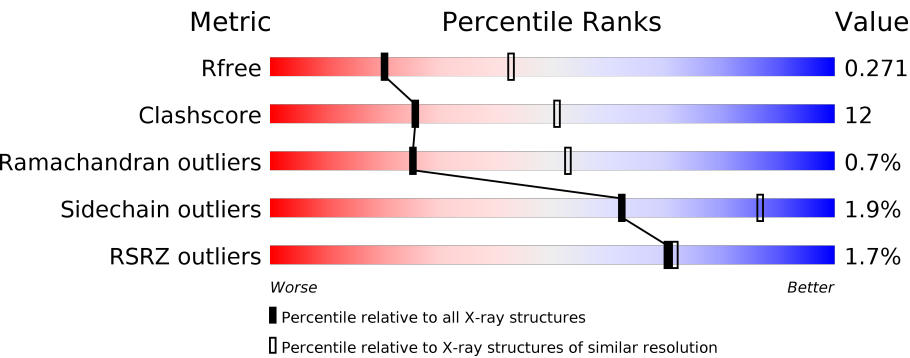
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	Y	15	<div><div>27%</div><div>60%33%7%</div></div>
1	Z	15	<div><div>27%</div><div>87%13%</div></div>
2	A	15	<div><div>20%</div><div>47%47%7%</div></div>
2	G	15	<div><div>27%</div><div>47%40%13%</div></div>
3	C	365	<div><div>70%25%. .</div></div>
3	E	365	<div><div>%73%22%.. .</div></div>

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Mol	Chain	Length	Quality of chain
3	I	365	
3	K	365	
4	D	37	
4	F	37	
4	J	37	
4	L	37	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MG	K	902	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14169 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 DNA chain called DNA (5'-D(\*GP\*GP\*TP\*CP\*GP\*GP\*TP\*GP\*AP\*CP\*CP\*GP\*AP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Y	15	Total	C	N	O	P	0	0	0
			306	145	59	88	14			
1	Z	15	Total	C	N	O	P	0	0	0
			306	145	59	88	14			

- Molecule 2 is a DNA chain called DNA (5'-D(\*GP\*GP\*TP\*CP\*GP\*GP\*TP\*CP\*AP\*CP\*CP\*GP\*AP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	15	Total	C	N	O	P	0	0	0
			303	144	57	88	14			
2	G	15	Total	C	N	O	P	0	0	0
			303	144	57	88	14			

- Molecule 3 is a protein called Probable DNA double-strand break repair Rad50 ATPase, Probable DNA double-strand break repair Rad50 ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	352	Total	C	N	O	S	256	0	0
			2824	1799	490	531	4			
3	E	351	Total	C	N	O	S	215	0	0
			2815	1794	489	528	4			
3	I	352	Total	C	N	O	S	211	0	0
			2824	1799	490	531	4			
3	K	352	Total	C	N	O	S	239	0	0
			2821	1797	490	530	4			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	676	SER	-	linker	UNP Q9X1X1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	677	SER	-	linker	UNP Q9X1X1
C	678	GLY	-	linker	UNP Q9X1X1
C	679	GLY	-	linker	UNP Q9X1X1
C	680	ALA	-	linker	UNP Q9X1X1
C	681	GLY	-	linker	UNP Q9X1X1
C	682	GLY	-	linker	UNP Q9X1X1
C	683	ALA	-	linker	UNP Q9X1X1
C	684	GLY	-	linker	UNP Q9X1X1
C	685	GLY	-	linker	UNP Q9X1X1
C	686	SER	-	linker	UNP Q9X1X1
E	676	SER	-	linker	UNP Q9X1X1
E	677	SER	-	linker	UNP Q9X1X1
E	678	GLY	-	linker	UNP Q9X1X1
E	679	GLY	-	linker	UNP Q9X1X1
E	680	ALA	-	linker	UNP Q9X1X1
E	681	GLY	-	linker	UNP Q9X1X1
E	682	GLY	-	linker	UNP Q9X1X1
E	683	ALA	-	linker	UNP Q9X1X1
E	684	GLY	-	linker	UNP Q9X1X1
E	685	GLY	-	linker	UNP Q9X1X1
E	686	SER	-	linker	UNP Q9X1X1
I	676	SER	-	linker	UNP Q9X1X1
I	677	SER	-	linker	UNP Q9X1X1
I	678	GLY	-	linker	UNP Q9X1X1
I	679	GLY	-	linker	UNP Q9X1X1
I	680	ALA	-	linker	UNP Q9X1X1
I	681	GLY	-	linker	UNP Q9X1X1
I	682	GLY	-	linker	UNP Q9X1X1
I	683	ALA	-	linker	UNP Q9X1X1
I	684	GLY	-	linker	UNP Q9X1X1
I	685	GLY	-	linker	UNP Q9X1X1
I	686	SER	-	linker	UNP Q9X1X1
K	189	SER	-	linker	UNP Q9X1X1
K	677	SER	-	linker	UNP Q9X1X1
K	678	GLY	-	linker	UNP Q9X1X1
K	679	GLY	-	linker	UNP Q9X1X1
K	680	ALA	-	linker	UNP Q9X1X1
K	681	GLY	-	linker	UNP Q9X1X1
K	682	GLY	-	linker	UNP Q9X1X1
K	683	ALA	-	linker	UNP Q9X1X1
K	684	GLY	-	linker	UNP Q9X1X1
K	685	GLY	-	linker	UNP Q9X1X1

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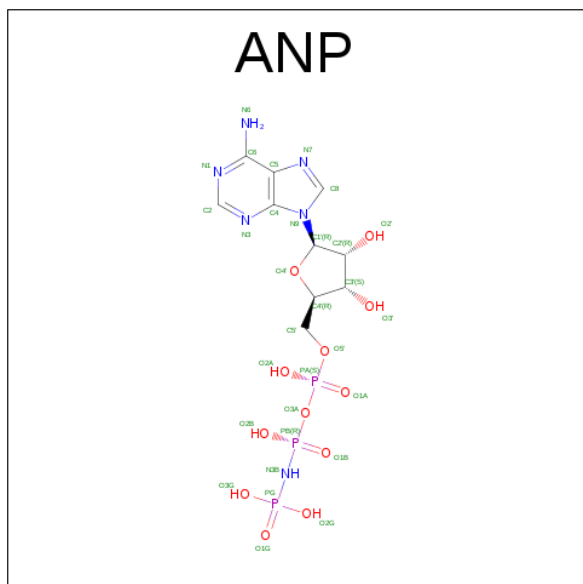
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Chain	Residue	Modelled	Actual	Comment	Reference
K	686	SER	-	linker	UNP Q9X1X1

- Molecule 4 is a protein called Exonuclease, putative.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	36	Total	C	N	O	81	0	0
			319	209	50	60			
4	F	36	Total	C	N	O	82	0	0
			321	210	50	61			
4	J	36	Total	C	N	O	83	0	0
			319	209	50	60			
4	L	35	Total	C	N	O	102	0	0
			313	206	49	58			

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	I	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	K	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	K	1	Total 1	Mg 1	0	0
6	I	1	Total 1	Mg 1	0	0
6	C	1	Total 1	Mg 1	0	0
6	E	1	Total 1	Mg 1	0	0

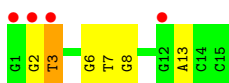
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	Y	2	Total 2	O 2	0	0
7	C	64	Total 64	O 64	0	0
7	D	1	Total 1	O 1	0	0
7	E	63	Total 63	O 63	0	0
7	F	1	Total 1	O 1	0	0
7	G	1	Total 1	O 1	0	0
7	I	67	Total 67	O 67	0	0
7	J	2	Total 2	O 2	0	0
7	K	63	Total 63	O 63	0	0
7	L	3	Total 3	O 3	0	0

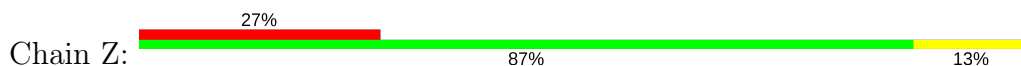
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

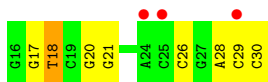
- Molecule 1: DNA (5'-D(\*GP\*GP\*TP\*CP\*GP\*GP\*TP\*GP\*AP\*CP\*CP\*GP\*AP\*CP\*C)-3')



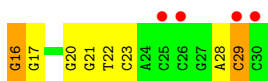
- Molecule 1: DNA (5'-D(\*GP\*GP\*TP\*CP\*GP\*GP\*TP\*GP\*AP\*CP\*CP\*GP\*AP\*CP\*C)-3')



- Molecule 2: DNA (5'-D(\*GP\*GP\*TP\*CP\*GP\*GP\*TP\*CP\*AP\*CP\*CP\*GP\*AP\*CP\*C)-3')



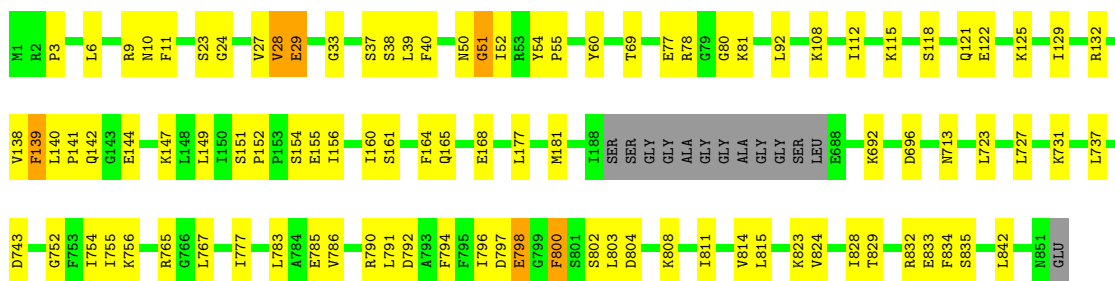
- Molecule 2: DNA (5'-D(\*GP\*GP\*TP\*CP\*GP\*GP\*TP\*CP\*AP\*CP\*CP\*GP\*AP\*CP\*C)-3')



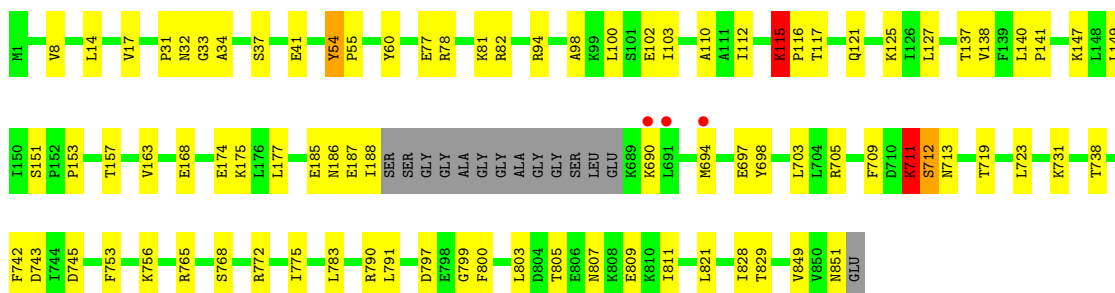
- Molecule 3: Probable DNA double-strand break repair Rad50 ATPase, Probable DNA double-strand break repair Rad50 ATPase



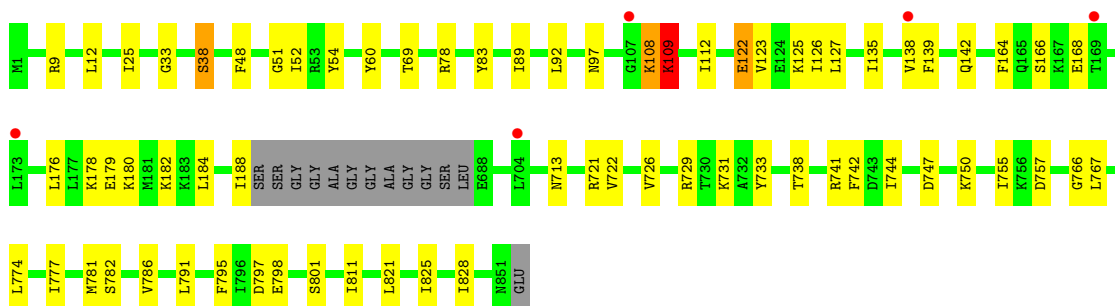
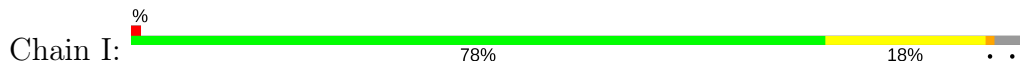




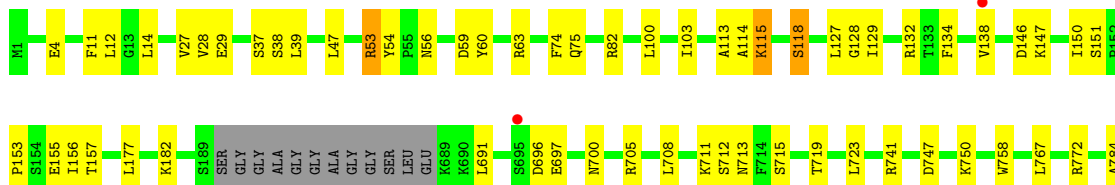
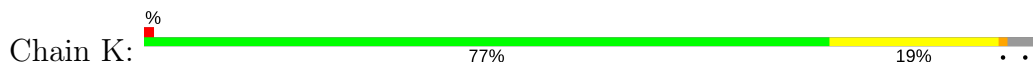
- Molecule 3: Probable DNA double-strand break repair Rad50 ATPase, Probable DNA double-strand break repair Rad50 ATPase



- Molecule 3: Probable DNA double-strand break repair Rad50 ATPase, Probable DNA double-strand break repair Rad50 ATPase



- Molecule 3: Probable DNA double-strand break repair Rad50 ATPase, Probable DNA double-strand break repair Rad50 ATPase





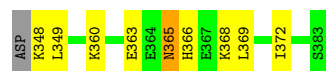
- Molecule 4: Exonuclease, putative



- Molecule 4: Exonuclease, putative



- Molecule 4: Exonuclease, putative



- Molecule 4: Exonuclease, putative



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.71Å 96.39Å 105.93Å 90.01° 89.22° 81.67°	Depositor
Resolution (Å)	47.69 – 2.70 47.68 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.3 (47.69-2.70) 92.4 (47.68-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.215 , 0.270 0.215 , 0.271	Depositor DCC
$R_{free}$ test set	2571 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.5	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 29.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.368 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	14169	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	Y	0.55	0/343	1.18	3/528 (0.6%)
1	Z	0.61	0/343	1.23	2/528 (0.4%)
2	A	0.54	0/339	1.26	2/521 (0.4%)
2	G	0.58	0/339	1.34	3/521 (0.6%)
3	C	0.49	1/2865 (0.0%)	0.65	5/3840 (0.1%)
3	E	0.61	5/2856 (0.2%)	0.77	6/3828 (0.2%)
3	I	0.64	2/2865 (0.1%)	0.87	4/3840 (0.1%)
3	K	0.54	0/2862	0.66	0/3836
4	D	0.29	0/323	0.42	0/427
4	F	0.31	0/325	0.49	0/430
4	J	0.31	0/323	0.45	0/427
4	L	0.31	0/317	0.54	0/419
All	All	0.56	8/14100 (0.1%)	0.80	25/19145 (0.1%)

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
3	E	0	3
3	I	0	1
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	108	LYS	C-N	-20.86	0.86	1.34
3	I	109	LYS	C-N	-7.37	1.17	1.34
3	E	54	TYR	CE1-CZ	-7.04	1.29	1.38
3	E	711	LYS	C-N	-5.65	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	28	VAL	C-N	-5.48	1.21	1.34
3	E	55	PRO	N-CD	5.31	1.55	1.47
3	E	54	TYR	CG-CD2	-5.14	1.32	1.39
3	E	116	PRO	N-CD	5.14	1.55	1.47

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	109	LYS	O-C-N	-29.63	75.29	122.70
3	I	109	LYS	CA-C-N	19.99	161.17	117.20
3	E	712	SER	O-C-N	-13.39	101.28	122.70
3	I	109	LYS	C-N-CA	12.67	153.38	121.70
3	E	711	LYS	O-C-N	-12.37	102.91	122.70
3	E	712	SER	CA-C-N	9.58	138.27	117.20
3	E	711	LYS	CA-C-N	8.22	135.28	117.20
3	E	712	SER	C-N-CA	8.06	141.86	121.70
3	C	28	VAL	O-C-N	-7.49	110.72	122.70
3	C	28	VAL	C-N-CA	7.01	139.23	121.70
2	G	20	DG	O4'-C1'-N9	5.98	112.19	108.00
2	G	16	DG	O4'-C1'-N9	5.88	112.11	108.00
3	E	115	LYS	C-N-CD	5.70	140.38	128.40
1	Y	13	DA	C1'-O4'-C4'	-5.68	104.42	110.10
3	C	52	ILE	N-CA-C	-5.63	95.79	111.00
2	A	18	DT	N3-C4-O4	5.54	123.23	119.90
2	G	29	DC	O4'-C1'-N1	5.54	111.88	108.00
3	C	29	GLU	O-C-N	-5.51	113.83	123.20
3	C	28	VAL	CA-C-N	5.37	129.00	117.20
1	Y	3	DT	O4'-C1'-N1	5.25	111.67	108.00
2	A	18	DT	C5-C4-O4	-5.23	121.24	124.90
1	Y	13	DA	O4'-C1'-N9	5.22	111.66	108.00
3	I	108	LYS	O-C-N	-5.08	114.58	122.70
1	Z	3	DT	O4'-C1'-N1	5.07	111.55	108.00
1	Z	13	DA	O4'-C1'-N9	5.03	111.52	108.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	711	LYS	Mainchain,Peptide
3	E	799	GLY	Peptide
3	I	109	LYS	Mainchain

## 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	Y	306	0	169	5	0
1	Z	306	0	169	0	0
2	A	303	0	169	4	1
2	G	303	0	169	5	0
3	C	2824	0	2891	82	4
3	E	2815	0	2886	57	3
3	I	2824	0	2891	61	0
3	K	2821	0	2891	57	0
4	D	319	0	332	1	0
4	F	321	0	331	5	0
4	J	319	0	332	7	0
4	L	313	0	327	7	0
5	C	31	0	13	2	0
5	E	31	0	13	3	0
5	I	31	0	13	2	0
5	K	31	0	13	1	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	I	1	0	0	0	0
6	K	1	0	0	0	0
7	C	64	0	0	7	0
7	D	1	0	0	0	0
7	E	63	0	0	8	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
7	I	67	0	0	8	0
7	J	2	0	0	0	0
7	K	63	0	0	9	0
7	L	3	0	0	0	0
7	Y	2	0	0	0	0
All	All	14169	0	13609	286	4

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 12.

All (286) 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)
3:I:108:LYS:C	3:I:109:LYS:CA	2.11	1.18
3:I:108:LYS:O	3:I:109:LYS:N	1.77	1.16
3:C:142:GLN:HG3	3:C:798:GLU:CB	1.79	1.13
3:I:798:GLU:CD	7:I:1036:HOH:O	1.86	1.10
3:I:108:LYS:CA	3:I:109:LYS:N	2.14	1.08
3:I:142:GLN:HG3	3:I:798:GLU:HB3	1.34	1.08
3:E:711:LYS:N	3:E:712:SER:HB2	1.69	1.07
3:I:798:GLU:OE2	7:I:1036:HOH:O	1.66	1.06
3:C:51:GLY:HA3	3:C:60:TYR:OH	1.59	1.01
3:K:772:ARG:NH2	7:K:1060:HOH:O	1.91	1.01
3:C:142:GLN:HG3	3:C:798:GLU:HB2	1.42	0.97
3:C:51:GLY:HA3	3:C:60:TYR:CZ	1.98	0.97
3:C:142:GLN:HG3	3:C:798:GLU:CG	1.94	0.96
3:K:829:THR:HG22	3:K:831:ASP:H	1.32	0.95
3:I:142:GLN:HG3	3:I:798:GLU:CB	1.99	0.92
3:E:8:VAL:HG11	3:E:14:LEU:HD12	1.49	0.92
3:C:33:GLY:H	5:C:901:ANP:HNB1	1.17	0.91
3:I:12:LEU:HD12	3:I:38:SER:HA	1.51	0.91
3:I:108:LYS:C	3:I:109:LYS:N	0.86	0.91
3:I:78:ARG:O	7:I:1013:HOH:O	1.86	0.90
3:E:731:LYS:NZ	3:E:745:ASP:OD1	2.07	0.87
3:K:27:VAL:HG11	3:K:835:SER:HB2	1.58	0.86
3:K:146:ASP:O	3:K:150:ILE:HG12	1.77	0.84
3:E:33:GLY:H	5:E:901:ANP:HNB1	1.22	0.84
3:I:821:LEU:O	7:I:1052:HOH:O	1.97	0.82
3:K:829:THR:HG22	3:K:831:ASP:N	1.96	0.80
3:C:38:SER:OG	5:C:901:ANP:O1A	1.98	0.80
3:K:127:LEU:O	7:K:1014:HOH:O	2.00	0.79
3:E:137:THR:HB	3:E:783:LEU:HD23	1.66	0.78
3:E:753:PHE:O	7:E:1025:HOH:O	2.03	0.77
3:K:829:THR:HG23	7:K:1021:HOH:O	1.84	0.77
3:C:765:ARG:NH1	7:C:1048:HOH:O	2.16	0.77
3:C:142:GLN:HE21	3:C:798:GLU:HG3	1.48	0.76
3:C:794:PHE:CZ	3:C:796:ILE:HD11	2.20	0.76
3:K:82:ARG:HG2	3:K:103:ILE:HD12	1.67	0.75
3:C:142:GLN:NE2	3:C:798:GLU:HG3	2.02	0.74
3:E:711:LYS:CA	3:E:712:SER:HB2	2.17	0.73
3:K:696:ASP:O	7:K:1063:HOH:O	2.06	0.73
3:K:829:THR:CG2	3:K:831:ASP:H	2.02	0.73
3:E:177:LEU:HD21	3:E:705:ARG:HB2	1.71	0.72
3:C:737:LEU:HD21	3:C:814:VAL:HG11	1.72	0.71
3:E:127:LEU:O	7:E:1015:HOH:O	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:147:LYS:O	3:E:151:SER:OG	2.09	0.71
3:K:157:THR:HG22	3:K:719:THR:HG21	1.73	0.71
3:I:12:LEU:HB2	3:I:38:SER:HB3	1.72	0.70
3:C:800:PHE:HA	3:C:803:LEU:HD12	1.74	0.69
3:C:177:LEU:O	3:C:181:MET:HG3	1.93	0.68
3:C:51:GLY:HA3	3:C:60:TYR:CE2	2.28	0.68
3:C:144:GLU:O	7:C:1046:HOH:O	2.12	0.68
3:E:98:ALA:O	3:E:115:LYS:N	2.25	0.68
3:C:24:GLY:O	7:C:1019:HOH:O	2.12	0.67
4:J:363:GLU:O	4:J:366:HIS:ND1	2.19	0.67
3:E:33:GLY:N	5:E:901:ANP:HNB1	1.92	0.67
3:I:755:ILE:HG13	3:I:767:LEU:HD11	1.77	0.67
3:C:797:ASP:HB2	3:C:828:ILE:HD12	1.78	0.66
3:I:108:LYS:O	3:I:109:LYS:CA	2.35	0.66
3:C:752:GLY:O	3:C:754:ILE:HG12	1.95	0.66
3:C:142:GLN:HG3	3:C:798:GLU:HG3	1.75	0.65
3:E:157:THR:HG22	3:E:719:THR:HG21	1.77	0.65
3:C:77:GLU:OE2	3:C:80:GLY:N	2.30	0.65
3:C:142:GLN:CG	3:C:798:GLU:CG	2.74	0.64
3:C:3:PRO:HD2	3:C:824:VAL:HG21	1.80	0.64
3:C:9:ARG:NH1	3:C:69:THR:O	2.30	0.63
3:C:797:ASP:O	7:C:1024:HOH:O	2.14	0.63
3:K:63:ARG:NH2	7:K:1001:HOH:O	2.31	0.63
3:I:97:ASN:ND2	7:I:1060:HOH:O	2.31	0.62
3:C:78:ARG:NH1	3:C:790:ARG:O	2.32	0.62
3:I:12:LEU:CB	3:I:38:SER:HB3	2.29	0.62
3:E:187:GLU:O	3:E:188:ILE:HB	2.00	0.62
3:I:766:GLY:HA2	3:K:53:ARG:HD3	1.82	0.61
3:C:151:SER:OG	3:C:152:PRO:HD2	1.98	0.61
4:J:348:LYS:O	4:J:349:LEU:HB2	2.01	0.61
3:I:731:LYS:NZ	3:I:744:ILE:O	2.33	0.60
3:K:37:SER:OG	3:K:797:ASP:OD2	2.19	0.60
3:C:692:LYS:O	3:C:696:ASP:CB	2.50	0.60
3:I:38:SER:OG	5:I:901:ANP:O1A	2.16	0.60
3:K:151:SER:OG	7:K:1059:HOH:O	2.12	0.60
3:E:703:LEU:HD23	4:F:369:LEU:HD11	1.84	0.60
3:C:785:GLU:OE2	7:C:1049:HOH:O	2.16	0.59
3:K:12:LEU:HD22	3:K:53:ARG:HH11	1.67	0.59
3:C:142:GLN:CG	3:C:798:GLU:HG3	2.31	0.59
3:K:12:LEU:HD12	3:K:38:SER:HA	1.85	0.59
3:I:176:LEU:HA	3:I:179:GLU:CG	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:PHE:CE2	3:C:60:TYR:HB3	2.38	0.58
3:K:177:LEU:HD21	3:K:705:ARG:HB2	1.84	0.58
3:E:78:ARG:NE	7:E:1015:HOH:O	2.31	0.58
3:E:765:ARG:NH1	7:E:1021:HOH:O	2.10	0.57
1:Y:7:DT:H2"	1:Y:8:DG:H8	1.69	0.57
3:C:692:LYS:O	3:C:696:ASP:HB3	2.05	0.57
3:E:149:LEU:O	7:E:1013:HOH:O	2.17	0.57
3:I:176:LEU:HA	3:I:179:GLU:HG2	1.85	0.57
3:I:12:LEU:CD1	3:I:38:SER:HA	2.30	0.57
3:E:117:THR:O	3:E:121:GLN:HG3	2.05	0.57
3:I:142:GLN:CG	3:I:798:GLU:HB3	2.22	0.57
3:E:711:LYS:H	3:E:712:SER:HB2	1.62	0.56
3:I:747:ASP:HB3	3:I:750:LYS:HB2	1.86	0.56
3:C:27:VAL:HG11	3:C:835:SER:HB2	1.87	0.56
3:I:184:LEU:O	3:I:188:ILE:HG13	2.05	0.56
3:I:797:ASP:OD1	3:I:828:ILE:HB	2.05	0.56
3:K:114:ALA:O	3:K:115:LYS:HB2	2.06	0.56
2:A:28:DA:H2"	2:A:29:DC:C6	2.40	0.56
3:C:160:ILE:HG23	3:C:783:LEU:HD21	1.88	0.55
1:Y:2:DG:N2	2:A:30:DC:O2	2.39	0.55
3:I:801:SER:HB2	3:K:801:SER:HB3	1.88	0.55
4:J:348:LYS:O	4:J:349:LEU:CB	2.55	0.55
3:C:51:GLY:CA	3:C:60:TYR:OH	2.45	0.55
3:I:54:TYR:HB2	3:I:60:TYR:CE1	2.42	0.55
3:I:729:ARG:HB3	3:I:782:SER:HB3	1.88	0.55
4:F:359:LEU:O	4:F:363:GLU:N	2.40	0.55
3:C:149:LEU:O	7:C:1025:HOH:O	2.18	0.54
3:K:12:LEU:HD22	3:K:53:ARG:NH1	2.23	0.54
3:I:108:LYS:O	3:I:109:LYS:HA	2.08	0.54
4:J:365:ASN:O	4:J:369:LEU:HG	2.07	0.53
3:C:777:ILE:HG21	3:C:811:ILE:HD11	1.89	0.53
3:K:711:LYS:O	3:K:715:SER:HB3	2.09	0.53
3:C:142:GLN:NE2	3:C:798:GLU:CG	2.71	0.53
3:C:755:ILE:HG13	3:C:767:LEU:HD11	1.90	0.53
3:C:737:LEU:CD2	3:C:814:VAL:HG11	2.39	0.53
3:K:115:LYS:HB2	3:K:118:SER:OG	2.09	0.52
3:E:803:LEU:CD1	3:E:811:ILE:HG13	2.40	0.52
3:C:142:GLN:CG	3:C:798:GLU:HB2	2.28	0.52
2:A:20:DG:H2"	2:A:21:DG:C8	2.45	0.52
3:K:700:ASN:HB2	7:K:1063:HOH:O	2.09	0.52
3:K:147:LYS:HA	3:K:150:ILE:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:83:TYR:CE2	3:I:126:ILE:HD13	2.45	0.52
3:K:56:ASN:HB3	3:K:59:ASP:OD2	2.10	0.52
3:I:48:PHE:CZ	3:I:127:LEU:HD12	2.44	0.51
3:I:797:ASP:OD1	3:I:828:ILE:CG2	2.58	0.51
3:K:12:LEU:CD1	3:K:38:SER:HA	2.41	0.51
3:E:78:ARG:HG3	3:E:78:ARG:HH11	1.74	0.51
3:K:11:PHE:CE1	3:K:60:TYR:HB3	2.45	0.51
3:C:727:LEU:O	3:C:731:LYS:HG3	2.11	0.51
3:E:743:ASP:HB3	3:E:756:LYS:HB2	1.92	0.51
3:E:775:ILE:HG22	3:E:775:ILE:O	2.11	0.51
3:I:721:ARG:HD3	7:I:1040:HOH:O	2.10	0.51
3:K:54:TYR:HB2	3:K:60:TYR:CE2	2.46	0.51
3:E:803:LEU:HD13	3:E:811:ILE:HG13	1.93	0.51
2:G:16:DG:H2''	2:G:17:DG:C8	2.46	0.51
3:C:125:LYS:HG2	3:C:168:GLU:HG2	1.92	0.50
4:F:352:PHE:O	4:F:356:LYS:N	2.37	0.50
4:L:377:LEU:O	4:L:381:LYS:N	2.44	0.50
2:A:17:DG:H1'	2:A:18:DT:H5'	1.93	0.50
4:L:381:LYS:O	4:L:382:LYS:C	2.49	0.50
3:I:12:LEU:HD12	3:I:38:SER:CA	2.33	0.50
3:E:100:LEU:CD2	3:E:112:ILE:HD12	2.41	0.50
2:G:22:DT:H2''	2:G:23:DC:C5	2.47	0.50
3:I:51:GLY:O	3:I:52:ILE:HD13	2.13	0.49
4:L:359:LEU:O	4:L:362:ARG:N	2.34	0.49
3:K:741:ARG:HD2	3:K:758:TRP:NE1	2.27	0.49
3:K:132:ARG:HH12	3:K:155:GLU:HG2	1.77	0.49
3:E:78:ARG:NH2	7:E:1015:HOH:O	2.46	0.49
2:G:28:DA:H2''	2:G:29:DC:C6	2.48	0.49
3:I:178:LYS:O	3:I:182:LYS:HB2	2.13	0.49
3:C:161:SER:O	3:C:165:GLN:HG2	2.13	0.49
3:C:40:PHE:CD1	3:C:40:PHE:C	2.86	0.49
3:E:790:ARG:NE	7:E:1034:HOH:O	2.13	0.49
3:I:176:LEU:CA	3:I:179:GLU:HG2	2.42	0.49
4:J:368:LYS:O	4:J:372:ILE:HG13	2.13	0.49
3:K:82:ARG:CG	3:K:103:ILE:HD12	2.41	0.49
3:K:697:GLU:HA	7:K:1063:HOH:O	2.13	0.48
3:E:32:ASN:ND2	5:E:901:ANP:O2G	2.43	0.48
3:E:738:THR:HG21	3:E:742:PHE:HD2	1.78	0.48
3:E:17:VAL:HG22	3:E:849:VAL:HG23	1.95	0.48
3:I:741:ARG:NH2	3:I:757:ASP:OD2	2.47	0.48
3:C:115:LYS:HE3	3:C:115:LYS:HB2	1.58	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:LEU:HD23	3:C:39:LEU:HD11	1.96	0.48
3:E:31:PRO:HG2	3:E:34:ALA:HB2	1.96	0.48
1:Y:7:DT:H2"	1:Y:8:DG:C8	2.46	0.47
3:I:777:ILE:O	3:I:781:MET:HG3	2.13	0.47
4:L:363:GLU:HG3	4:L:365:ASN:H	1.80	0.47
3:C:156:ILE:O	3:C:160:ILE:HG13	2.15	0.47
3:E:807:ASN:O	3:E:811:ILE:HG12	2.13	0.47
3:C:832:ARG:HG2	3:C:832:ARG:NH1	2.29	0.47
3:K:797:ASP:HA	3:K:828:ILE:HB	1.95	0.47
3:E:54:TYR:HB2	3:E:60:TYR:CZ	2.50	0.47
3:E:711:LYS:CA	3:E:712:SER:CB	2.89	0.47
3:K:153:PRO:O	3:K:157:THR:HG23	2.15	0.47
3:E:102:GLU:N	3:E:110:ALA:O	2.44	0.47
3:E:102:GLU:HG3	3:E:103:ILE:N	2.28	0.47
3:K:829:THR:HG22	3:K:830:HIS:N	2.29	0.46
3:C:154:SER:HB2	7:C:1061:HOH:O	2.16	0.46
3:K:4:GLU:HB2	3:K:75:GLN:HG2	1.97	0.46
3:I:9:ARG:NH1	3:I:69:THR:O	2.48	0.46
3:C:743:ASP:HB3	3:C:756:LYS:HB2	1.97	0.46
3:K:47:LEU:HD21	3:K:74:PHE:CE2	2.50	0.46
3:C:132:ARG:HH12	3:C:155:GLU:HG2	1.81	0.46
3:K:147:LYS:O	3:K:151:SER:OG	2.31	0.46
3:C:692:LYS:O	3:C:696:ASP:N	2.45	0.46
3:C:800:PHE:N	3:C:800:PHE:CD1	2.84	0.46
3:C:9:ARG:HD2	3:C:10:ASN:OD1	2.16	0.46
3:E:138:VAL:HG21	3:E:791:LEU:HD13	1.97	0.46
1:Y:2:DG:C2	1:Y:3:DT:C2	3.04	0.46
4:F:354:LEU:HD23	4:F:354:LEU:HA	1.85	0.45
3:K:28:VAL:HB	3:K:828:ILE:HG12	1.98	0.45
4:D:377:LEU:HA	4:D:377:LEU:HD23	1.85	0.45
3:I:33:GLY:H	5:I:901:ANP:HNB1	1.62	0.45
3:E:37:SER:O	3:E:41:GLU:HG3	2.17	0.45
3:E:723:LEU:HD23	3:E:723:LEU:HA	1.72	0.45
3:C:11:PHE:CZ	3:C:60:TYR:CD2	3.04	0.45
3:C:138:VAL:HG21	3:C:791:LEU:HD13	1.97	0.45
3:E:174:GLU:HB2	3:E:709:PHE:CE1	2.52	0.45
3:I:138:VAL:HG21	3:I:791:LEU:HD13	1.97	0.45
4:F:376:LEU:O	4:F:380:VAL:HG23	2.17	0.45
2:G:21:DG:H2"	2:G:22:DT:C6	2.51	0.45
3:I:112:ILE:HG22	3:I:122:GLU:HG3	1.98	0.45
3:C:800:PHE:HE2	3:C:815:LEU:HD11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:185:GLU:HG3	3:E:698:TYR:CE2	2.52	0.45
3:K:14:LEU:HD11	3:K:39:LEU:HD13	2.00	0.44
3:E:797:ASP:HA	3:E:828:ILE:HB	1.98	0.44
3:K:100:LEU:N	3:K:113:ALA:O	2.33	0.44
3:C:40:PHE:CZ	3:C:139:PHE:CD2	3.06	0.44
3:K:29:GLU:HA	3:K:829:THR:O	2.18	0.44
3:E:140:LEU:HA	3:E:141:PRO:HD3	1.79	0.44
3:C:129:ILE:HD13	3:C:791:LEU:HD11	2.00	0.43
3:K:128:GLY:O	7:K:1017:HOH:O	2.21	0.43
3:C:54:TYR:HB2	3:C:60:TYR:CE1	2.53	0.43
4:J:360:LYS:HG2	4:J:366:HIS:CD2	2.53	0.43
3:C:28:VAL:HG22	3:C:842:LEU:HD23	2.00	0.43
3:C:164:PHE:CZ	3:C:786:VAL:HG12	2.53	0.43
1:Y:6:DG:H2"	1:Y:7:DT:C6	2.54	0.43
3:C:140:LEU:HA	3:C:141:PRO:HD3	1.76	0.43
4:J:349:LEU:HD12	4:J:349:LEU:HA	1.76	0.43
3:E:138:VAL:CG2	3:E:791:LEU:HD13	2.49	0.43
3:I:25:ILE:HA	3:I:825:ILE:O	2.18	0.43
3:C:29:GLU:HA	3:C:829:THR:O	2.18	0.43
3:C:829:THR:CG2	3:C:835:SER:HB3	2.48	0.43
3:E:8:VAL:CG1	3:E:14:LEU:HD12	2.34	0.43
3:I:176:LEU:O	3:I:180:LYS:HG3	2.19	0.43
3:C:121:GLN:O	3:C:125:LYS:HG3	2.19	0.43
3:E:153:PRO:O	3:E:157:THR:HG23	2.19	0.43
3:E:8:VAL:HG11	3:E:14:LEU:CD1	2.35	0.43
3:K:829:THR:CG2	3:K:830:HIS:N	2.82	0.43
3:E:163:VAL:O	3:E:790:ARG:HD3	2.19	0.42
3:I:166:SER:N	7:I:1062:HOH:O	2.48	0.42
3:K:182:LYS:HD2	3:K:182:LYS:HA	1.89	0.42
3:I:176:LEU:C	3:I:179:GLU:HG2	2.39	0.42
3:I:774:LEU:HA	3:I:811:ILE:HD11	2.01	0.42
3:K:47:LEU:HD21	3:K:74:PHE:HE2	1.83	0.42
4:L:359:LEU:O	4:L:363:GLU:N	2.49	0.42
3:C:37:SER:OG	3:C:797:ASP:OD2	2.36	0.42
3:I:164:PHE:CZ	3:I:786:VAL:HG12	2.54	0.42
3:K:708:LEU:HD13	4:L:355:PHE:CE1	2.54	0.42
3:E:125:LYS:HD2	7:E:1052:HOH:O	2.19	0.42
3:E:768:SER:O	3:E:772:ARG:HB2	2.20	0.42
3:I:729:ARG:HA	3:I:729:ARG:HD2	1.70	0.42
3:I:797:ASP:CG	3:I:828:ILE:HD12	2.40	0.42
3:C:54:TYR:HA	3:C:55:PRO:HD3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:791:LEU:HD23	3:E:791:LEU:HA	1.76	0.42
2:G:16:DG:H2''	2:G:17:DG:H8	1.83	0.42
3:K:151:SER:O	3:K:156:ILE:HD11	2.20	0.42
3:K:723:LEU:HD23	3:K:723:LEU:HA	1.78	0.42
3:C:723:LEU:HD23	3:C:723:LEU:HA	1.85	0.42
3:C:92:LEU:HD23	3:C:92:LEU:HA	1.78	0.42
3:K:37:SER:HB2	5:K:901:ANP:O1A	2.20	0.42
3:K:794:PHE:O	3:K:825:ILE:HA	2.19	0.42
3:C:112:ILE:HG22	3:C:122:GLU:HG3	2.01	0.41
3:C:147:LYS:O	3:C:151:SER:HB2	2.20	0.41
3:I:125:LYS:HG3	3:I:168:GLU:HG2	2.02	0.41
3:K:129:ILE:HD11	3:K:134:PHE:HD1	1.85	0.41
3:E:82:ARG:HG2	3:E:103:ILE:HD12	2.02	0.41
3:K:151:SER:O	3:K:156:ILE:CD1	2.68	0.41
3:C:808:LYS:HD3	3:C:834:PHE:HB2	2.03	0.41
3:K:747:ASP:HB3	3:K:750:LYS:HB2	2.02	0.41
3:E:77:GLU:HG2	3:E:81:LYS:O	2.20	0.41
3:I:127:LEU:HA	3:I:127:LEU:HD23	1.89	0.41
3:I:738:THR:HG21	3:I:742:PHE:HD2	1.85	0.41
3:I:797:ASP:OD1	3:I:828:ILE:CB	2.68	0.41
3:E:805:THR:O	3:E:809:GLU:HG3	2.20	0.41
3:C:115:LYS:HB2	3:C:118:SER:OG	2.20	0.41
3:C:164:PHE:HZ	3:C:786:VAL:HG12	1.85	0.41
3:E:78:ARG:CG	3:E:78:ARG:HH11	2.34	0.41
3:I:166:SER:HB3	7:I:1062:HOH:O	2.20	0.41
3:I:139:PHE:CD1	3:I:795:PHE:HB2	2.56	0.41
3:C:23:SER:HA	3:C:823:LYS:O	2.21	0.41
3:E:690:LYS:O	3:E:694:MET:HG3	2.21	0.41
3:I:722:VAL:O	3:I:726:VAL:HG23	2.20	0.41
3:K:75:GLN:NE2	3:K:82:ARG:HD3	2.36	0.41
3:C:832:ARG:HH11	3:C:832:ARG:HG2	1.86	0.40
3:K:138:VAL:HG12	3:K:784:ALA:HB2	2.02	0.40
3:C:125:LYS:HG2	3:C:168:GLU:CG	2.51	0.40
3:C:792:ASP:HA	3:C:823:LYS:HE3	2.02	0.40
3:C:832:ARG:CG	3:C:832:ARG:HH11	2.35	0.40
3:I:729:ARG:NH2	3:I:733:TYR:CZ	2.90	0.40
3:C:77:GLU:HG2	3:C:81:LYS:O	2.21	0.40
4:L:368:LYS:O	4:L:372:ILE:HG13	2.22	0.40
3:I:122:GLU:O	3:I:126:ILE:HG13	2.22	0.40

All (4) 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)
3:C:833:GLU:N	3:E:94:ARG:NH2[1_455]	1.87	0.33
3:C:833:GLU:N	3:E:94:ARG:NH1[1_455]	1.93	0.27
2:A:26:DC:OP2	3:C:108:LYS:NZ[1_655]	2.00	0.20
3:C:833:GLU:N	3:E:94:ARG:CZ[1_455]	2.10	0.10

## 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	
3	C	348/365 (95%)	327 (94%)	17 (5%)	4 (1%)	17	40
3	E	347/365 (95%)	331 (95%)	14 (4%)	2 (1%)	28	56
3	I	348/365 (95%)	329 (94%)	18 (5%)	1 (0%)	44	73
3	K	348/365 (95%)	325 (93%)	19 (6%)	4 (1%)	17	40
4	D	34/37 (92%)	32 (94%)	2 (6%)	0	100	100
4	F	34/37 (92%)	32 (94%)	2 (6%)	0	100	100
4	J	34/37 (92%)	32 (94%)	2 (6%)	0	100	100
4	L	33/37 (89%)	29 (88%)	4 (12%)	0	100	100
All	All	1526/1608 (95%)	1437 (94%)	78 (5%)	11 (1%)	25	53

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	713	ASN
3	K	712	SER
3	C	51	GLY
3	C	713	ASN
3	K	713	ASN
3	I	713	ASN
3	K	115	LYS
3	K	767	LEU
3	C	798	GLU

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Mol	Chain	Res	Type
3	C	804	ASP
3	E	115	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	306/311 (98%)	302 (99%)	4 (1%)	73	91
3	E	305/311 (98%)	297 (97%)	8 (3%)	51	81
3	I	306/311 (98%)	300 (98%)	6 (2%)	60	86
3	K	306/311 (98%)	300 (98%)	6 (2%)	60	86
4	D	36/37 (97%)	36 (100%)	0	100	100
4	F	36/37 (97%)	35 (97%)	1 (3%)	49	79
4	J	36/37 (97%)	35 (97%)	1 (3%)	49	79
4	L	35/37 (95%)	35 (100%)	0	100	100
All	All	1366/1392 (98%)	1340 (98%)	26 (2%)	62	87

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	50	ASN
3	C	139	PHE
3	C	800	PHE
3	C	802	SER
3	E	168	GLU
3	E	175	LYS
3	E	186	ASN
3	E	697	GLU
3	E	800	PHE
3	E	821	LEU
3	E	829	THR
3	E	851	ASN
4	F	378	ASP

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Mol	Chain	Res	Type
3	I	38	SER
3	I	89	ILE
3	I	92	LEU
3	I	122	GLU
3	I	123	VAL
3	I	135	ILE
4	J	365	ASN
3	K	53	ARG
3	K	118	SER
3	K	691	LEU
3	K	806	GLU
3	K	835	SER
3	K	844	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	50	ASN
3	E	75	GLN
3	E	830	HIS
4	L	365	ASN

### 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, 4 are monoatomic - leaving 4 for Mogul analysis.



In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	ANP	C	901	6	29,33,33	2.88	5 (17%)	28,52,52	0.87	1 (3%)
5	ANP	E	901	6	29,33,33	1.95	5 (17%)	28,52,52	1.22	3 (10%)
5	ANP	I	901	6	29,33,33	2.44	2 (6%)	28,52,52	1.39	3 (10%)
5	ANP	K	901	6	29,33,33	1.99	5 (17%)	28,52,52	1.24	3 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ANP	C	901	6	-	0/13/38/38	0/3/3/3
5	ANP	E	901	6	-	0/13/38/38	0/3/3/3
5	ANP	I	901	6	-	0/13/38/38	0/3/3/3
5	ANP	K	901	6	-	0/13/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	901	ANP	PB-O2B	-3.17	1.48	1.56
5	C	901	ANP	PG-O3G	-2.85	1.48	1.56
5	E	901	ANP	PB-O2B	-2.84	1.48	1.56
5	C	901	ANP	PB-O3A	-2.78	1.55	1.59
5	C	901	ANP	PB-O2B	-2.76	1.49	1.56
5	I	901	ANP	PG-O3G	-2.61	1.49	1.56
5	E	901	ANP	PG-N3B	2.62	1.70	1.63
5	E	901	ANP	PB-N3B	2.69	1.70	1.63
5	K	901	ANP	PB-N3B	2.80	1.70	1.63
5	K	901	ANP	PG-N3B	2.83	1.70	1.63
5	E	901	ANP	PG-O1G	3.20	1.49	1.46
5	K	901	ANP	PG-O1G	3.22	1.49	1.46
5	E	901	ANP	PB-O1B	8.10	1.55	1.46
5	K	901	ANP	PB-O1B	8.20	1.55	1.46
5	C	901	ANP	PB-O1B	8.91	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	901	ANP	PG-O1G	11.12	1.58	1.46
5	I	901	ANP	PG-O1G	12.21	1.60	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	901	ANP	O1B-PB-N3B	-4.54	105.00	111.79
5	K	901	ANP	O3G-PG-O1G	-3.19	105.29	113.41
5	E	901	ANP	O2G-PG-O1G	-3.14	105.43	113.41
5	E	901	ANP	O3G-PG-O1G	-3.08	105.57	113.41
5	K	901	ANP	O1B-PB-N3B	-2.80	107.61	111.79
5	K	901	ANP	O1G-PG-N3B	-2.54	107.99	111.79
5	I	901	ANP	O2G-PG-O1G	-2.09	108.09	113.41
5	C	901	ANP	O2G-PG-O1G	-2.00	108.32	113.41
5	E	901	ANP	O3G-PG-O2G	2.12	113.63	107.69
5	I	901	ANP	O1G-PG-N3B	3.36	116.81	111.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	901	ANP	2	0
5	E	901	ANP	3	0
5	I	901	ANP	2	0
5	K	901	ANP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	I	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	109:LYS	C	110:ALA	N	1.17
1	I	108:LYS	C	109:LYS	N	0.86

## 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	Y	15/15 (100%)	1.76	4 (26%) 1 0	136, 158, 186, 194	0
1	Z	15/15 (100%)	1.86	4 (26%) 1 0	122, 146, 183, 183	0
2	A	15/15 (100%)	1.02	3 (20%) 1 1	75, 140, 176, 177	0
2	G	15/15 (100%)	1.00	4 (26%) 1 0	64, 132, 167, 167	0
3	C	352/365 (96%)	-0.19	0 100 100	17, 29, 62, 82	94 (26%)
3	E	351/365 (96%)	-0.16	3 (0%) 84 85	17, 28, 59, 73	78 (22%)
3	I	352/365 (96%)	-0.15	5 (1%) 75 76	18, 29, 55, 89	67 (19%)
3	K	352/365 (96%)	-0.14	4 (1%) 80 81	16, 27, 57, 80	78 (22%)
4	D	36/37 (97%)	-0.42	0 100 100	41, 57, 72, 75	23 (63%)
4	F	36/37 (97%)	-0.46	0 100 100	43, 61, 74, 79	22 (61%)
4	J	36/37 (97%)	-0.45	0 100 100	36, 51, 65, 67	20 (55%)
4	L	35/37 (94%)	-0.35	0 100 100	45, 66, 80, 82	27 (77%)
All	All	1610/1668 (96%)	-0.12	27 (1%) 70 72	16, 30, 75, 194	409 (25%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Z	1	DG	6.1
1	Y	2	DG	5.9
1	Y	1	DG	4.7
1	Z	2	DG	4.7
1	Z	4	DC	4.3
2	A	25	DC	4.2
1	Z	3	DT	4.0
3	E	690	LYS	3.7
3	K	695	SER	3.6
1	Y	12	DG	3.3
3	I	107	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	A	24	DA	3.2
1	Y	3	DT	3.2
2	G	29	DC	3.0
3	I	173	LEU	2.9
3	I	169	THR	2.7
3	K	796	ILE	2.5
3	E	691	LEU	2.4
3	I	704	LEU	2.4
3	E	694	MET	2.3
2	A	29	DC	2.2
3	K	834	PHE	2.2
2	G	26	DC	2.2
2	G	30	DC	2.2
2	G	25	DC	2.1
3	I	138	VAL	2.0
3	K	138	VAL	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
6	MG	K	902	1/1	0.99	0.21	2.17	13,13,13,13	0
5	ANP	I	901	31/31	0.97	0.17	0.16	15,19,24,24	0
5	ANP	C	901	31/31	0.97	0.15	-0.28	14,19,22,23	0
5	ANP	K	901	31/31	0.97	0.16	-0.41	11,19,23,26	0
5	ANP	E	901	31/31	0.97	0.15	-0.77	11,19,23,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	E	902	1/1	0.97	0.14	-0.89	14,14,14,14	0
6	MG	I	902	1/1	0.96	0.14	-1.09	16,16,16,16	0
6	MG	C	902	1/1	0.96	0.13	-1.51	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.