



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 05:50 PM BST

PDB ID : 6KCO  
Title : Shuguo PWWP in complex with ssDNA  
Authors : Liu, Y.C.; Huang, Y.  
Deposited on : 2019-06-28  
Resolution : 2.40 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

<https://www.wwpdb.org/validation/2017/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  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

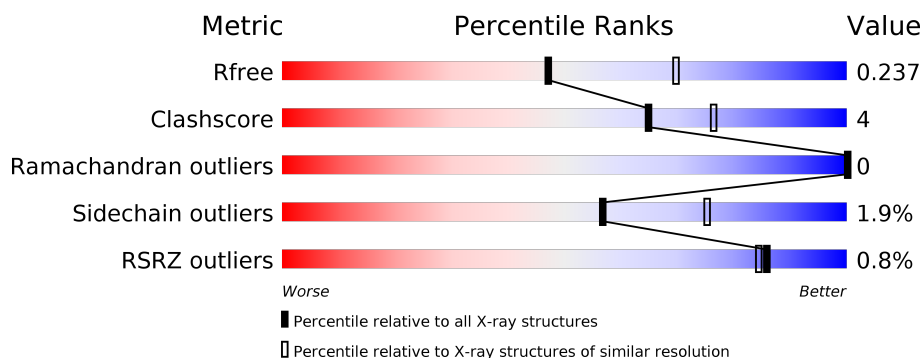
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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.













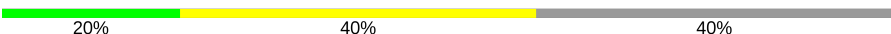
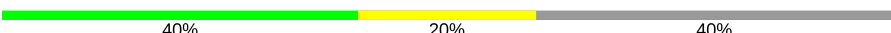
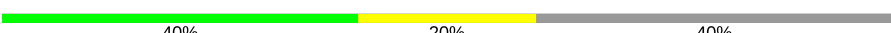

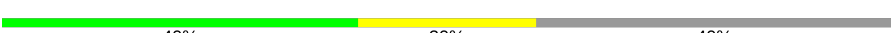





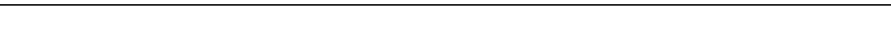
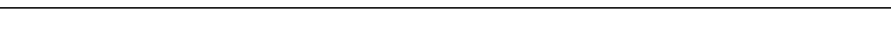

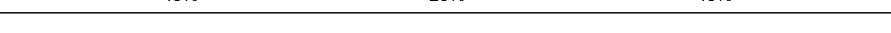
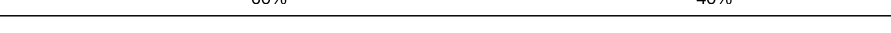
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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	85	<div> <div>86%</div> <div>11%</div> <div>••</div> </div>
1	B	85	<div>2%</div> <div>85%</div> <div>13%</div> <div>•</div>


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Mol	Chain	Length	Quality of chain
1	G	85	
1	H	85	
1	I	85	
1	J	85	
1	K	85	
1	L	85	
1	M	85	
1	N	85	
1	O	85	
1	P	85	
2	1H	5	
2	1O	5	
2	1P	5	
2	2G	5	
2	2M	5	
2	3B	5	
2	3L	5	
2	4D	5	
2	4J	5	
2	5I	5	
2	6A	5	
2	6F	5	
2	7C	5	
2	7E	5	
2	8K	5	

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Mol	Chain	Length	Quality of chain
2	9N	5	 <div>60%40%</div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11761 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 LD23804p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	83	Total	C	N	O	S	0	0	0
			662	432	108	121	1			
1	B	83	Total	C	N	O	S	0	0	0
			662	432	108	121	1			
1	C	81	Total	C	N	O	S	0	0	0
			650	426	104	119	1			
1	D	82	Total	C	N	O	S	0	0	0
			663	432	109	121	1			
1	E	81	Total	C	N	O	S	0	0	0
			646	423	103	119	1			
1	F	83	Total	C	N	O	S	0	0	0
			668	435	110	122	1			
1	G	80	Total	C	N	O	S	0	0	0
			651	426	106	118	1			
1	H	81	Total	C	N	O	S	0	0	0
			655	427	107	120	1			
1	I	80	Total	C	N	O	S	0	0	0
			645	423	103	118	1			
1	J	82	Total	C	N	O	S	0	0	0
			656	428	107	120	1			
1	K	80	Total	C	N	O	S	0	0	0
			645	423	103	118	1			
1	L	80	Total	C	N	O	S	0	0	0
			645	423	103	118	1			
1	M	82	Total	C	N	O	S	0	0	0
			661	431	107	122	1			
1	N	83	Total	C	N	O	S	0	0	0
			665	434	109	121	1			
1	O	80	Total	C	N	O	S	0	0	0
			641	420	102	118	1			
1	P	81	Total	C	N	O	S	0	0	0
			656	429	107	119	1			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	SER	-	expression tag	UNP Q9VAA9
B	7	SER	-	expression tag	UNP Q9VAA9
C	7	SER	-	expression tag	UNP Q9VAA9
D	7	SER	-	expression tag	UNP Q9VAA9
E	7	SER	-	expression tag	UNP Q9VAA9
F	7	SER	-	expression tag	UNP Q9VAA9
G	7	SER	-	expression tag	UNP Q9VAA9
H	7	SER	-	expression tag	UNP Q9VAA9
I	7	SER	-	expression tag	UNP Q9VAA9
J	7	SER	-	expression tag	UNP Q9VAA9
K	7	SER	-	expression tag	UNP Q9VAA9
L	7	SER	-	expression tag	UNP Q9VAA9
M	7	SER	-	expression tag	UNP Q9VAA9
N	7	SER	-	expression tag	UNP Q9VAA9
O	7	SER	-	expression tag	UNP Q9VAA9
P	7	SER	-	expression tag	UNP Q9VAA9

- Molecule 2 is a DNA chain called DNA (5'-D(\*TP\*CP\*CP\*CP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1O	3	Total	C	N	O	P	0	0	0
			48	24	5	17	2			
2	2M	3	Total	C	N	O	P	0	0	0
			47	24	6	15	2			
2	1P	3	Total	C	N	O	P	0	0	0
			40	19	5	14	2			
2	1H	3	Total	C	N	O	P	0	0	0
			40	19	5	14	2			
2	4D	3	Total	C	N	O	P	0	0	0
			48	24	6	16	2			
2	7E	3	Total	C	N	O	P	0	0	0
			46	24	5	15	2			
2	6F	5	Total	C	N	O	P	0	0	0
			88	42	12	29	5			
2	2G	4	Total	C	N	O	P	0	0	0
			51	24	5	19	3			
2	5I	4	Total	C	N	O	P	0	0	0
			52	24	6	19	3			
2	4J	3	Total	C	N	O	P	0	0	0
			48	24	6	16	2			
2	3L	3	Total	C	N	O	P	0	0	0
			54	28	8	16	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9N	3	Total	C	N	O	P	0	0	0
			47	24	5	16	2			
2	6A	3	Total	C	N	O	P	0	0	0
			48	24	6	16	2			
2	3B	4	Total	C	N	O	P	0	0	0
			59	28	8	20	3			
2	7C	3	Total	C	N	O	P	0	0	0
			55	28	8	17	2			
2	8K	3	Total	C	N	O	P	0	0	0
			40	19	5	14	2			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	27	Total	O	0	0
			27	27		
3	C	40	Total	O	0	0
			40	40		
3	D	24	Total	O	0	0
			24	24		
3	E	42	Total	O	0	0
			42	42		
3	F	42	Total	O	0	0
			42	42		
3	G	6	Total	O	0	0
			6	6		
3	H	21	Total	O	0	0
			21	21		
3	I	28	Total	O	0	0
			28	28		
3	J	27	Total	O	0	0
			27	27		
3	K	17	Total	O	0	0
			17	17		
3	L	31	Total	O	0	0
			31	31		
3	M	33	Total	O	0	0
			33	33		
3	N	37	Total	O	0	0
			37	37		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	26	Total 26	O 26	0	0
3	P	19	Total 19	O 19	0	0
3	1O	2	Total 2	O 2	0	0
3	2M	3	Total 3	O 3	0	0
3	1P	2	Total 2	O 2	0	0
3	1H	4	Total 4	O 4	0	0
3	4D	1	Total 1	O 1	0	0
3	7E	5	Total 5	O 5	0	0
3	6F	3	Total 3	O 3	0	0
3	2G	2	Total 2	O 2	0	0
3	5I	2	Total 2	O 2	0	0
3	4J	3	Total 3	O 3	0	0
3	3L	3	Total 3	O 3	0	0
3	9N	2	Total 2	O 2	0	0
3	6A	3	Total 3	O 3	0	0
3	3B	1	Total 1	O 1	0	0
3	7C	3	Total 3	O 3	0	0
3	8K	1	Total 1	O 1	0	0



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


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: LD23804p

Chain A:  86% 11% ..




#### • Molecule 1: LD23804p

Chain B:  85% 13% .




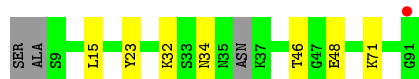
#### • Molecule 1: LD23804p

Chain C:  86% 9% 5%




#### • Molecule 1: LD23804p

Chain D:  88% 8% .




#### • Molecule 1: LD23804p

Chain E:  82% 13% 5%




#### • Molecule 1: LD23804p

Chain F:  88% 8% ..




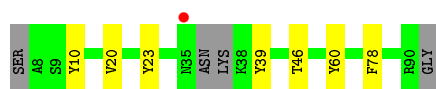
• Molecule 1: LD23804p

Chain G:  76% 15% • 6%




• Molecule 1: LD23804p

Chain H:  87% 8% 5%




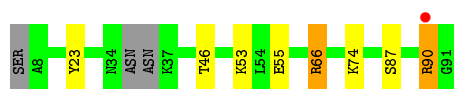
• Molecule 1: LD23804p

Chain I:  88% 6% 6%




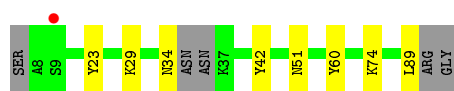
• Molecule 1: LD23804p

Chain J:  87% 7% • •




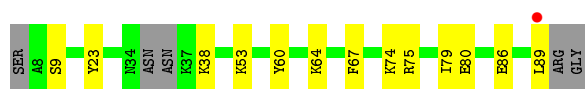
• Molecule 1: LD23804p

Chain K:  85% 9% 6%




• Molecule 1: LD23804p

Chain L:  79% 15% 6%




• Molecule 1: LD23804p

Chain M:  84% 13%




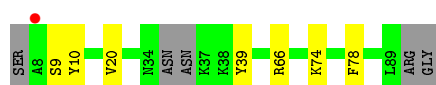
- Molecule 1: LD23804p

Chain N:  87% 11%




- Molecule 1: LD23804p

Chain O:  86% 8% 6%



- Molecule 1: LD23804p

Chain P:  80% 14% 5%



- Molecule 2: DNA (5'-D(\*TP\*CP\*CP\*CP\*T)-3')

Chain 1O:  40% 20% 40%



- Molecule 2: DNA (5'-D(\*TP\*CP\*CP\*CP\*T)-3')

Chain 2M:  40% 20% 40%

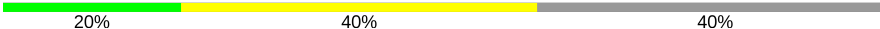


- Molecule 2: DNA (5'-D(\*TP\*CP\*CP\*CP\*T)-3')

Chain 1P:  40% 20% 40%



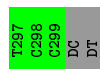
- Molecule 2: DNA (5'-D(\*TP\*CP\*CP\*CP\*T)-3')

Chain 1H: 



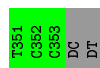
- Molecule 2: DNA (5'-D(\*TP\*CP\*CP\*CP\*T)-3')

Chain 4D: 



- Molecule 2: DNA (5'-D(\*TP\*CP\*CP\*CP\*T)-3')

Chain 7E: 




- Molecule 2: DNA (5'-D(\*TP\*CP\*CP\*CP\*T)-3')

Chain 6F: 



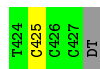
- Molecule 2: DNA (5'-D(\*TP\*CP\*CP\*CP\*T)-3')

Chain 2G: 



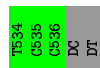
- Molecule 2: DNA (5'-D(\*TP\*CP\*CP\*CP\*T)-3')

Chain 5I: 



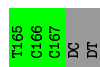
- Molecule 2: DNA (5'-D(\*TP\*CP\*CP\*CP\*T)-3')

Chain 4J: 

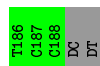


- Molecule 2: DNA (5'-D(\*TP\*CP\*CP\*CP\*T)-3')

Chain 3L: 



- Molecule 2: DNA (5'-D(\*TP\*CP\*CP\*CP\*T)-3')



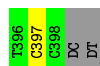
- Molecule 2: DNA (5'-D(\*TP\*CP\*CP\*CP\*T)-3')



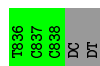
- Molecule 2: DNA (5'-D(\*TP\*CP\*CP\*CP\*T)-3')



- Molecule 2: DNA (5'-D(\*TP\*CP\*CP\*CP\*T)-3')



- Molecule 2: DNA (5'-D(\*TP\*CP\*CP\*CP\*T)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.67Å 76.33Å 85.26Å 101.75° 106.08° 113.75°	Depositor
Resolution (Å)	29.94 – 2.40 29.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.3 (29.94-2.40) 96.3 (29.94-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.198 , 0.236 0.199 , 0.237	Depositor DCC
$R_{free}$ test set	2009 reflections (3.65%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.1	Xtriage
Anisotropy	0.780	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 40.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11761	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% 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 ⓘ

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	0.26	0/678	0.41	0/914
1	B	0.26	0/678	0.44	0/914
1	C	0.26	0/665	0.42	0/894
1	D	0.25	0/678	0.43	0/910
1	E	0.32	0/661	0.43	0/890
1	F	0.45	1/683 (0.1%)	0.46	0/917
1	G	0.30	0/666	0.45	0/894
1	H	0.25	0/670	0.41	0/901
1	I	0.25	0/660	0.42	0/887
1	J	0.39	0/671	0.50	1/902 (0.1%)
1	K	0.26	0/660	0.41	0/887
1	L	0.26	0/660	0.42	0/887
1	M	0.26	0/677	0.42	0/912
1	N	0.26	0/680	0.43	0/913
1	O	0.26	0/656	0.42	0/883
1	P	0.26	0/670	0.42	0/898
2	1H	0.49	0/43	1.03	0/65
2	1O	0.43	0/51	0.93	0/76
2	1P	0.50	0/43	1.03	0/65
2	2G	0.56	0/55	1.01	0/83
2	2M	0.56	0/51	0.98	0/77
2	3B	0.56	0/64	0.99	0/97
2	3L	0.62	0/59	1.06	0/89
2	4D	0.46	0/52	0.96	0/78
2	4J	0.50	0/52	0.94	0/78
2	5I	0.53	0/56	1.03	0/85
2	6A	0.49	0/52	0.94	0/78
2	6F	0.49	0/96	0.89	0/144
2	7C	0.51	0/60	0.89	0/90
2	7E	0.57	0/50	1.00	0/75
2	8K	0.47	0/43	1.00	0/65
2	9N	0.58	0/51	1.00	0/76
All	All	0.31	1/11591 (0.0%)	0.50	1/15724 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	84	GLN	CG-CD	8.57	1.70	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	90	ARG	CA-CB-CG	5.32	125.09	113.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	662	0	658	8	0
1	B	662	0	658	9	0
1	C	650	0	653	10	0
1	D	663	0	668	5	0
1	E	646	0	642	12	0
1	F	668	0	673	7	0
1	G	651	0	659	12	0
1	H	655	0	657	7	0
1	I	645	0	651	4	0
1	J	656	0	656	8	0
1	K	645	0	651	6	0
1	L	645	0	651	8	0
1	M	661	0	664	6	0
1	N	665	0	669	8	1
1	O	641	0	640	4	0
1	P	656	0	660	7	0
2	1H	40	0	24	2	0
2	1O	48	0	31	1	0
2	1P	40	0	24	1	0
2	2G	51	0	30	0	0
2	2M	47	0	29	1	0
2	3B	59	0	35	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3L	54	0	33	0	0
2	4D	48	0	32	0	0
2	4J	48	0	32	0	0
2	5I	52	0	31	1	0
2	6A	48	0	32	1	0
2	6F	88	0	53	3	0
2	7C	55	0	36	1	0
2	7E	46	0	28	0	0
2	8K	40	0	24	0	0
2	9N	47	0	31	0	0
3	1H	4	0	0	0	0
3	1O	2	0	0	0	0
3	1P	2	0	0	0	0
3	2G	2	0	0	0	0
3	2M	3	0	0	0	0
3	3B	1	0	0	0	0
3	3L	3	0	0	0	0
3	4D	1	0	0	0	0
3	4J	3	0	0	0	0
3	5I	2	0	0	0	0
3	6A	3	0	0	0	0
3	6F	3	0	0	0	0
3	7C	3	0	0	0	0
3	7E	5	0	0	0	0
3	8K	1	0	0	0	0
3	9N	2	0	0	0	0
3	A	19	0	0	0	0
3	B	27	0	0	1	0
3	C	40	0	0	1	1
3	D	24	0	0	0	0
3	E	42	0	0	0	0
3	F	42	0	0	0	0
3	G	6	0	0	0	0
3	H	21	0	0	0	0
3	I	28	0	0	0	0
3	J	27	0	0	0	0
3	K	17	0	0	1	0
3	L	31	0	0	0	0
3	M	33	0	0	0	0
3	N	37	0	0	0	0
3	O	26	0	0	0	0
3	P	19	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11761	0	11015	91	1

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 4.

All (91) 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:44:TYR:HD1	1:F:84:GLN:OE1	1.59	0.84
1:E:32:LYS:NZ	1:E:34:ASN:OD1	2.18	0.76
1:C:13:GLY:O	3:C:101:HOH:O	2.11	0.69
1:P:51:ASN:N	3:P:102:HOH:O	2.28	0.66
1:E:44:TYR:CD1	1:F:84:GLN:HB3	2.31	0.66
1:E:44:TYR:CD1	1:F:84:GLN:OE1	2.47	0.65
1:K:29:LYS:NZ	3:K:101:HOH:O	2.29	0.65
1:A:66:ARG:HD2	1:G:66:ARG:HD2	1.78	0.65
1:G:33:SER:OG	1:G:37:LYS:NZ	2.31	0.64
1:G:74:LYS:HD2	1:H:23:TYR:CE2	2.33	0.62
1:L:80:GLU:HG3	1:N:91:GLY:HA3	1.80	0.62
1:A:74:LYS:NZ	1:B:22:GLY:O	2.34	0.61
1:B:8:ALA:N	3:B:101:HOH:O	2.35	0.59
1:K:29:LYS:HG2	1:K:42:TYR:HB3	1.85	0.58
1:I:23:TYR:CE2	1:J:74:LYS:HE2	2.39	0.57
1:G:77:LYS:HG2	1:H:46:THR:HG22	1.88	0.55
1:H:20:VAL:HG21	2:1H:177:DT:H1'	1.89	0.54
1:C:74:LYS:HE2	1:D:23:TYR:CE2	2.43	0.54
1:P:38:LYS:HG2	1:P:53:LYS:HA	1.88	0.54
1:C:48:GLU:HB3	2:6A:744:DC:C4	2.45	0.52
1:E:57:LEU:O	1:N:66:ARG:NH2	2.42	0.52
1:C:77:LYS:HG2	1:D:46:THR:HG22	1.92	0.52
1:K:23:TYR:CE2	1:L:74:LYS:HE2	2.45	0.51
1:E:48:GLU:HB3	2:1P:259:DC:C4	2.46	0.50
1:B:63:ASN:OD1	1:B:66:ARG:HD3	2.11	0.50
1:E:38:LYS:NZ	1:E:51:ASN:O	2.42	0.50
1:M:19:LYS:HD3	1:M:58:PHE:CE1	2.47	0.50
1:D:48:GLU:HB3	2:5I:425:DC:C4	2.47	0.49
1:K:60:TYR:OH	1:L:86:GLU:OE2	2.31	0.49
1:N:73:MET:HG2	2:6F:210:DT:H4'	1.93	0.49
1:O:10:TYR:HB2	1:O:39:TYR:CE2	2.47	0.49
1:G:89:LEU:HD11	1:H:60:TYR:HE2	1.78	0.48
1:G:32:LYS:NZ	1:G:34:ASN:OD1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:GLU:O	1:B:69:THR:HG23	2.14	0.48
1:C:89:LEU:HD13	1:D:15:LEU:HD12	1.94	0.48
1:G:71:LYS:HE3	1:H:78:PHE:CZ	2.48	0.48
1:I:74:LYS:HD3	1:J:23:TYR:CE2	2.48	0.48
1:E:66:ARG:NH2	1:N:57:LEU:O	2.46	0.47
1:C:66:ARG:HD2	1:J:66:ARG:HD2	1.95	0.47
1:J:53:LYS:NZ	1:J:55:GLU:OE1	2.47	0.47
1:A:48:GLU:HB3	2:7C:397:DC:C4	2.50	0.46
1:P:49:THR:O	3:P:101:HOH:O	2.20	0.46
1:N:77:LYS:HD2	1:N:77:LYS:HA	1.65	0.46
1:L:75:ARG:CZ	1:L:79:ILE:HD11	2.46	0.46
1:K:74:LYS:HD3	1:L:23:TYR:CE2	2.50	0.46
1:K:34:ASN:ND2	1:K:51:ASN:OD1	2.49	0.46
1:M:46:THR:HG21	2:2M:329:DT:O4	2.15	0.45
2:3B:126:DC:H3'	2:3B:127:DC:O2	2.16	0.45
1:E:44:TYR:HA	1:F:84:GLN:OE1	2.17	0.45
1:E:21:LYS:HG2	1:F:21:LYS:HG3	1.98	0.45
1:P:37:LYS:HE2	1:P:39:TYR:OH	2.17	0.45
1:J:87:SER:HA	1:J:90:ARG:HG2	1.98	0.44
1:N:70:GLU:HB3	1:N:74:LYS:HE2	1.98	0.44
1:C:70:GLU:O	1:C:74:LYS:HG3	2.16	0.44
1:C:66:ARG:CD	1:J:66:ARG:HD2	2.47	0.44
1:M:77:LYS:HD3	1:M:77:LYS:HA	1.85	0.44
1:N:77:LYS:HE2	2:6F:209:DC:O4'	2.18	0.44
1:M:34:ASN:ND2	1:M:51:ASN:OD1	2.51	0.44
1:G:89:LEU:HD11	1:H:60:TYR:CE2	2.53	0.43
1:F:80:GLU:O	1:F:83:ASP:N	2.43	0.43
1:M:48:GLU:HB3	2:6F:207:DC:C4	2.53	0.43
1:A:69:THR:O	1:A:73:MET:HG2	2.18	0.43
1:E:65:GLU:HB3	1:N:8:ALA:HB2	2.00	0.43
1:B:48:GLU:HB3	2:1H:178:DC:C4	2.52	0.43
1:A:89:LEU:HD13	1:B:15:LEU:HD12	2.01	0.43
1:P:42:TYR:CZ	1:P:47:GLY:HA2	2.54	0.43
1:D:32:LYS:HE2	1:D:34:ASN:OD1	2.19	0.43
1:H:10:TYR:HB2	1:H:39:TYR:CE2	2.54	0.43
1:G:12:ILE:H	1:G:12:ILE:HD12	1.83	0.43
1:G:19:LYS:HE2	1:G:58:PHE:CZ	2.53	0.43
1:I:66:ARG:HG3	1:I:67:PHE:N	2.33	0.43
1:L:38:LYS:HG2	1:L:53:LYS:HA	1.99	0.42
1:B:66:ARG:O	1:B:70:GLU:HG3	2.19	0.42
1:L:60:TYR:CE2	1:L:64:LYS:HE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:TYR:CZ	1:A:47:GLY:HA2	2.55	0.42
1:C:55:GLU:N	1:C:55:GLU:OE2	2.46	0.42
1:F:35:ASN:C	1:F:37:LYS:HG3	2.40	0.42
1:B:70:GLU:O	1:B:74:LYS:HG2	2.19	0.41
1:A:38:LYS:HE3	1:A:51:ASN:ND2	2.35	0.41
1:I:77:LYS:CD	1:J:46:THR:HG22	2.50	0.41
1:J:87:SER:HA	1:J:90:ARG:CG	2.50	0.41
1:G:42:TYR:CZ	1:G:47:GLY:HA2	2.55	0.41
1:E:12:ILE:HD12	1:E:12:ILE:H	1.85	0.41
1:L:75:ARG:O	1:L:79:ILE:HG12	2.20	0.41
1:C:66:ARG:O	1:C:70:GLU:HG3	2.21	0.41
1:O:20:VAL:HG21	2:1O:527:DT:H1'	2.02	0.41
1:O:74:LYS:HE3	1:P:23:TYR:CE2	2.55	0.41
1:O:78:PHE:CE2	1:P:71:LYS:HE2	2.56	0.41
1:A:74:LYS:HE3	1:B:23:TYR:CD2	2.56	0.40
1:G:37:LYS:HA	1:G:37:LYS:HD2	1.85	0.40
1:M:35:ASN:HB3	1:M:37:LYS:HE2	2.02	0.40

All (1) 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:N:75:ARG:NH2	3:C:101:HOH:O[1_556]	2.14	0.06

## 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	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
1	B	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
1	C	77/85 (91%)	77 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	78/85 (92%)	76 (97%)	2 (3%)	0	100	100
1	E	77/85 (91%)	76 (99%)	1 (1%)	0	100	100
1	F	79/85 (93%)	77 (98%)	2 (2%)	0	100	100
1	G	76/85 (89%)	76 (100%)	0	0	100	100
1	H	77/85 (91%)	76 (99%)	1 (1%)	0	100	100
1	I	76/85 (89%)	76 (100%)	0	0	100	100
1	J	78/85 (92%)	78 (100%)	0	0	100	100
1	K	76/85 (89%)	76 (100%)	0	0	100	100
1	L	76/85 (89%)	75 (99%)	1 (1%)	0	100	100
1	M	80/85 (94%)	78 (98%)	2 (2%)	0	100	100
1	N	79/85 (93%)	79 (100%)	0	0	100	100
1	O	76/85 (89%)	76 (100%)	0	0	100	100
1	P	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
All	All	1242/1360 (91%)	1229 (99%)	13 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	67/71 (94%)	66 (98%)	1 (2%)	65	80
1	B	67/71 (94%)	67 (100%)	0	100	100
1	C	67/71 (94%)	67 (100%)	0	100	100
1	D	69/71 (97%)	68 (99%)	1 (1%)	67	82
1	E	66/71 (93%)	66 (100%)	0	100	100
1	F	69/71 (97%)	67 (97%)	2 (3%)	42	62
1	G	68/71 (96%)	65 (96%)	3 (4%)	28	45
1	H	68/71 (96%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	67/71 (94%)	67 (100%)	0	100	100
1	J	67/71 (94%)	66 (98%)	1 (2%)	65	80
1	K	67/71 (94%)	66 (98%)	1 (2%)	65	80
1	L	67/71 (94%)	64 (96%)	3 (4%)	27	44
1	M	69/71 (97%)	67 (97%)	2 (3%)	42	62
1	N	68/71 (96%)	68 (100%)	0	100	100
1	O	66/71 (93%)	64 (97%)	2 (3%)	41	61
1	P	68/71 (96%)	64 (94%)	4 (6%)	19	32
All	All	1080/1136 (95%)	1060 (98%)	20 (2%)	57	75

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	D	71	LYS
1	F	9	SER
1	F	87	SER
1	G	9	SER
1	G	66	ARG
1	G	77	LYS
1	J	66	ARG
1	K	89	LEU
1	L	9	SER
1	L	67	PHE
1	L	89	LEU
1	M	9	SER
1	M	73	MET
1	O	9	SER
1	O	66	ARG
1	P	34	ASN
1	P	37	LYS
1	P	66	ARG
1	P	87	SER

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

Mol	Chain	Res	Type
1	L	34	ASN

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Mol	Chain	Res	Type
1	P	34	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	83/85 (97%)	-0.39	0 100 100	25, 35, 47, 63	0
1	B	83/85 (97%)	-0.20	2 (2%) 59 57	24, 32, 49, 64	0
1	C	81/85 (95%)	-0.36	0 100 100	22, 29, 43, 53	0
1	D	82/85 (96%)	-0.30	1 (1%) 79 77	22, 31, 47, 70	0
1	E	81/85 (95%)	-0.53	0 100 100	22, 29, 41, 50	0
1	F	83/85 (97%)	-0.46	0 100 100	20, 28, 40, 59	0
1	G	80/85 (94%)	-0.19	0 100 100	28, 37, 50, 67	0
1	H	81/85 (95%)	-0.18	1 (1%) 79 77	26, 36, 52, 61	0
1	I	80/85 (94%)	-0.20	1 (1%) 77 75	21, 28, 44, 51	0
1	J	82/85 (96%)	-0.36	1 (1%) 79 77	23, 30, 46, 57	0
1	K	80/85 (94%)	-0.27	1 (1%) 77 75	24, 32, 48, 50	0
1	L	80/85 (94%)	-0.33	1 (1%) 77 75	22, 29, 41, 53	0
1	M	82/85 (96%)	-0.38	0 100 100	20, 28, 41, 48	0
1	N	83/85 (97%)	-0.41	1 (1%) 79 77	21, 29, 41, 57	0
1	O	80/85 (94%)	-0.00	1 (1%) 77 75	25, 33, 45, 50	0
1	P	81/85 (95%)	-0.24	1 (1%) 79 77	24, 34, 52, 65	0
2	1H	3/5 (60%)	-1.09	0 100 100	29, 29, 32, 35	0
2	1O	3/5 (60%)	-0.49	0 100 100	27, 27, 34, 58	0
2	1P	3/5 (60%)	-0.96	0 100 100	28, 28, 32, 42	0
2	2G	4/5 (80%)	-0.12	0 100 100	30, 32, 55, 81	0
2	2M	3/5 (60%)	-0.63	0 100 100	24, 24, 26, 41	0
2	3B	4/5 (80%)	-0.22	0 100 100	29, 29, 43, 60	0
2	3L	3/5 (60%)	-0.06	0 100 100	28, 28, 31, 61	0
2	4D	3/5 (60%)	-0.64	0 100 100	28, 28, 33, 55	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
2	4J	3/5 (60%)	0.01	0	100	100	29, 29, 29, 53	0
2	5I	4/5 (80%)	-0.35	0	100	100	25, 28, 45, 70	0
2	6A	3/5 (60%)	-0.35	0	100	100	29, 29, 32, 48	0
2	6F	5/5 (100%)	0.39	0	100	100	25, 26, 61, 63	0
2	7C	3/5 (60%)	-0.21	0	100	100	27, 27, 29, 65	0
2	7E	3/5 (60%)	-0.91	0	100	100	27, 27, 27, 43	0
2	8K	3/5 (60%)	-0.52	0	100	100	27, 27, 30, 38	0
2	9N	3/5 (60%)	-0.73	0	100	100	25, 25, 27, 46	0
All	All	1355/1440 (94%)	-0.30	11 (0%)	86	84	20, 32, 49, 81	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	36	ASN	4.2
1	J	90	ARG	3.7
1	L	89	LEU	3.6
1	P	8	ALA	3.4
1	D	91	GLY	3.3
1	K	9	SER	2.8
1	O	8	ALA	2.5
1	I	9	SER	2.4
1	B	33	SER	2.2
1	N	35	ASN	2.2
1	H	35	ASN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.