

wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 – 10:10 PM EST

PDB ID	:	8UK9
Title	:	Structure of T4 Bacteriophage clamp loader mutant D110C bound to the T4
		clamp, primer-template DNA, and ATP analog
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Deposited on	:	2023-10-12
Resolution	:	3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
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)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.10 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)	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(Å)}) \end{array}$
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 of 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 <=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 a	chain	
1	А	187	52%	36%	8% • •
1	Q	187	18%	37%	10% ••
2	В	320	67%	30%	•
2	С	320	69%	28%	•
2	D	320	60%	36%	•••

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Mol	Chain	Length	Quality of chain						
2	Е	320	53%	40% 6% ·					
2	К	320	4% 65%	31% •					
2	L	320	65%	32% •					
2	М	320	59%	37% •••					
2	Ν	320	53%	35% 7% 5%					
3	F	228	54%	39% 7%					
3	G	228	<u>2</u> % 7 5%	22% ·					
3	Н	228	4% 73%	26% •					
3	R	228	<u>8%</u> 68%	31% •					
3	S	228	62%	36% •					
3	Т	228	66%	29% •					
4	Ι	24	33%	67%					
4	О	24	29%	71%					
5	J	20	40%	60%					
5	Р	20	55%	45%					

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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	AF3	В	901	-	-	Х	-
6	AF3	Κ	402	-	-	Х	-
6	AF3	L	402	-	-	Х	-
6	AF3	М	402	-	-	Х	-



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 35422 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	100	Total	С	Ν	Ο	\mathbf{S}	0	1	0
1	A	162	1474	951	242	275	6	0		0
1	0	183	Total	С	Ν	0	S	0	0	0
1	I Q		1469	947	244	272	6	0	0	0

• Molecule 1 is a protein called Sliding-clamp-loader small subunit.

• Molecule 2 is a protein called Sliding-clamp-loader large subunit.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	р	310	Total	С	Ν	0	S	0	0	0
	D	519	2507	1586	431	472	18	0	0	0
0	C	300	Total	С	Ν	0	S	0	0	0
		320	2513	1589	432	474	18	0	0	0
9	П	318	Total	С	Ν	0	S	0	0	0
	D	510	2499	1581	430	471	17	0	0	0
9	F	318	Total	С	Ν	Ο	S	0	0	0
	Ľ		2499	1581	430	471	17	0	0	0
9	K	310	Total	С	Ν	0	S	0	0	0
	Γ	519	2507	1586	431	472	18	0	0	0
2	T	320	Total	С	Ν	Ο	\mathbf{S}	0	0	0
2		520	2513	1589	432	474	18	0	0	0
2	М	317	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	111	517	2492	1578	426	470	18	0	0	0
2	N	305	Total	С	Ν	0	S	0	0	0
	1	305	2407	1526	413	451	17	0		0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	0	SER	-	expression tag	UNP P04526
В	110	CYS	ASP	engineered mutation	UNP P04526
С	0	SER	-	expression tag	UNP P04526
С	110	CYS	ASP	engineered mutation	UNP P04526
D	0	SER	-	expression tag	UNP P04526

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Defenence	1

Chain	Residue	Modelled	Actual	Comment	Reference
D	110	CYS	ASP	engineered mutation	UNP P04526
E	0	SER	-	expression tag	UNP P04526
Е	110	CYS	ASP	engineered mutation	UNP P04526
K	0	SER	-	expression tag	UNP P04526
K	110	CYS	ASP	engineered mutation	UNP P04526
L	0	SER	-	expression tag	UNP P04526
L	110	CYS	ASP	engineered mutation	UNP P04526
М	0	SER	-	expression tag	UNP P04526
М	110	CYS	ASP	engineered mutation	UNP P04526
N	0	SER	-	expression tag	UNP P04526
N	110	CYS	ASP	engineered mutation	UNP P04526

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• Molecule 3 is a protein called Sliding clamp.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	2 F	228	Total	С	Ν	0	S	0	0	0
0	Г	220	1750	1113	288	343	6	0	0	0
9	C	222	Total	С	Ν	0	S	0	0	0
0	G	220	1750	1113	288	343	6	0	0	0
9	п	222	Total	С	Ν	0	S	0	0	0
0	п	220	1750	1113	288	343	6	0	0	0
9	D	222	Total	С	Ν	0	S	0	0	0
0	n	220	1750	1113	288	343	6	0	0	0
9	C	222	Total	С	Ν	0	S	0	0	0
Ð	3 5	228	1750	1113	288	343	6	0	0	0
9		220	Total	С	Ν	0	S	0	0	0
0		220	1750	1113	288	343	6		U	U

• Molecule 4 is a DNA chain called DNA template.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
4	т	24	Total	С	Ν	Ο	Р	0	0	0
4	1	24	489	236	76	153	24			
4	0	24	Total	С	Ν	0	Р	0	0	0
4	4 0		489	236	76	153	24			0

• Molecule 5 is a DNA chain called DNA primer.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
5	J	20	Total 408	C 195	N 81	0 113	Р 19	0	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
5	Р	20	Total 408	C 195	N 81	0 113	Р 19	0	0	0

• Molecule 6 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	Total Al F 4 1 3	0	0
6	С	1	TotalAlF413	0	0
6	D	1	Total Al F 4 1 3	0	0
6	Κ	1	Total Al F 4 1 3	0	0
6	L	1	Total Al F 4 1 3	0	0
6	М	1	TotalAlF413	0	0

• Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	В	1	Total	С	Ν	Ο	Р	0	0
1	D	1	27	10	5	10	2	0	0
7	С	1	Total	С	Ν	Ο	Р	0	0
1	U		27	10	5	10	2	0	0
7	Л	1	Total	С	Ν	Ο	Р	0	0
1	D	1	27	10	5	10	2	0	0
7	F	1	Total	С	Ν	Ο	Р	0	0
1	Ľ	1	27	10	5	10	2	0	0
7	K	1	Total	С	Ν	Ο	Р	0	0
1	Т	1	27	10	5	10	2	0	0
7	т	1	Total	С	Ν	Ο	Р	0	0
1	L	1	27	10	5	10	2	0	0
7	М	1	Total	С	Ν	Ο	Р	0	0
	111	I	27	10	5	10	2	0	U
7	Ν	1	Total	С	Ν	Ο	Р	0	Ο
1	1	1 I	27	10	5	10	2	0	

• Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	В	1	Total Mg 1 1	0	0
8	С	1	Total Mg 1 1	0	0
8	D	1	Total Mg 1 1	0	0
8	Е	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	K	1	Total Mg 1 1	0	0
8	L	1	Total Mg 1 1	0	0
8	М	1	Total Mg 1 1	0	0
8	Ν	1	Total Mg 1 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: Sliding-clamp-loader small subunit

• Molecule 1: Sliding-clamp-loader small subunit





• Molecule 2: Sliding-clamp-loader large subunit



• Molecule 2: Sliding-clamp-loader large subunit



• Molecule 2: Sliding-clamp-loader large subunit



• Molecule 2: Sliding-clamp-loader large subunit









• Molecule 4: 1	DNA template	
Chain I:	33%	67%
110 110 1110 1113 1110 1118 1110 1118 1110 1110	121 723 123 124 124 126 126 128 128 128 128 128 128 128 128 128	
• Molecule 4: 1	DNA template	
Chain O:	29%	71%
T7 T8 T19 T11 A12 A16 A16 C17 C17 C17	C19 721 721 724 724 726 726 726 726 726 726 726 727	
• Molecule 5:	DNA primer	
Chain J:	40%	60%
61 64 73 73 73 73 74 75 74 75 74 70 74 70 74 70 74 70 74 70 74 70 75 74 70 75 74 70 75 75 75 75 75 75 75 75 75 75 75 75 75	612 613 720 A20	
• Molecule 5:	DNA primer	
Chain P:	55%	45%
G1 C2 G4 A3 A5 C6 A18 A18 A19 A19 A19 A20		



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	95.24Å 231.99Å 264.51Å	Dopositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	48.13 - 3.10	Depositor
Resolution (A)	48.13 - 3.10	EDS
% Data completeness	71.3 (48.13-3.10)	Depositor
(in resolution range)	71.3(48.13-3.10)	EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.69 (at 3.12 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
P. P.	0.253 , 0.265	Depositor
n, n_{free}	0.253 , 0.264	DCC
R_{free} test set	1999 reflections (2.62%)	wwPDB-VP
Wilson B-factor $(Å^2)$	95.1	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.22, 39.4	EDS
L-test for $twinning^2$	$ < L >=0.45, < L^2>=0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	35422	wwPDB-VP
Average B, all atoms $(Å^2)$	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: MG, ADP, AF3 $\,$

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).

Mal	Chain	Bond	lengths	Bond	angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.24	0/1505	0.45	0/2025
1	Q	0.27	0/1495	0.48	0/2011
2	В	0.27	0/2551	0.47	0/3438
2	С	0.24	0/2557	0.47	0/3446
2	D	0.26	0/2543	0.48	0/3428
2	Е	0.29	0/2543	0.52	0/3428
2	Κ	0.25	0/2551	0.48	0/3438
2	L	0.25	0/2557	0.47	0/3446
2	М	0.25	0/2535	0.47	0/3416
2	N	0.25	0/2450	0.49	0/3300
3	F	0.25	0/1779	0.48	0/2410
3	G	0.25	0/1779	0.46	0/2410
3	Н	0.25	0/1779	0.45	0/2410
3	R	0.25	0/1779	0.49	0/2410
3	S	0.25	0/1779	0.47	0/2410
3	Т	0.25	0/1779	0.51	0/2410
4	Ι	0.53	0/544	1.07	0/838
4	0	0.51	0/544	1.04	0/838
5	J	0.50	0/459	0.85	0/706
5	Р	0.48	0/459	0.82	0/706
All	All	0.28	0/35967	0.52	0/48924

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
2	Κ	0	1
3	Т	0	1
All	All	0	2



There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Κ	21	ASP	Peptide
3	Т	148	VAL	Peptide

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	А	1474	0	1491	61	0
1	Q	1469	0	1502	60	0
2	В	2507	0	2538	76	0
2	С	2513	0	2543	72	0
2	D	2499	0	2526	98	0
2	Е	2499	0	2523	147	0
2	K	2507	0	2539	76	0
2	L	2513	0	2543	80	0
2	М	2492	0	2521	91	0
2	N	2407	0	2434	95	0
3	F	1750	0	1755	77	0
3	G	1750	0	1755	34	0
3	Н	1750	0	1755	33	0
3	R	1750	0	1755	51	0
3	S	1750	0	1755	59	0
3	Т	1750	0	1755	52	0
4	Ι	489	0	277	17	0
4	0	489	0	277	17	0
5	J	408	0	225	10	0
5	Р	408	0	225	10	0
6	В	4	0	0	4	0
6	С	4	0	0	1	0
6	D	4	0	0	0	0
6	K	4	0	0	2	0
6	L	4	0	0	2	0
6	М	4	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	В	27	0	12	8	0
7	С	27	0	12	6	0
7	D	27	0	12	5	0
7	Е	27	0	12	6	0
7	Κ	27	0	12	4	0
7	L	27	0	12	4	0
7	М	27	0	12	8	0
7	Ν	27	0	12	5	0
8	В	1	0	0	0	0
8	С	1	0	0	0	0
8	D	1	0	0	0	0
8	Е	1	0	0	0	0
8	Κ	1	0	0	0	0
8	L	1	0	0	0	0
8	М	1	0	0	0	0
8	Ν	1	0	0	0	0
All	All	35422	0	34790	1084	0

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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 16.

The worst 5 of 1084 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)
2:E:250:LEU:HD22	2:E:309:PHE:HB3	1.41	1.02
3:F:190:GLN:HB3	3:F:191:PRO:HD2	1.46	0.96
2:C:145:ILE:HG13	2:C:147:PRO:HD2	1.52	0.92
2:L:12:GLU:OE2	2:M:153:ARG:NH1	2.08	0.85
1:A:134:ASN:HD22	2:E:111:ARG:NH2	1.74	0.85

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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentile
1	А	179/187~(96%)	142 (79%)	21 (12%)	16~(9%)	1 4
1	Q	179/187~(96%)	140 (78%)	28 (16%)	11 (6%)	1 9
2	В	317/320~(99%)	291 (92%)	19 (6%)	7~(2%)	6 29
2	С	318/320~(99%)	290 (91%)	22~(7%)	6(2%)	8 33
2	D	316/320~(99%)	287~(91%)	20~(6%)	9~(3%)	5 25
2	Ε	316/320~(99%)	281 (89%)	26~(8%)	9~(3%)	5 25
2	Κ	317/320~(99%)	289 (91%)	21 (7%)	7~(2%)	6 29
2	L	318/320~(99%)	286 (90%)	25~(8%)	7~(2%)	6 29
2	М	313/320~(98%)	289 (92%)	23~(7%)	1 (0%)	41 73
2	Ν	301/320~(94%)	266 (88%)	32 (11%)	3~(1%)	15 49
3	F	226/228~(99%)	181 (80%)	37~(16%)	8 (4%)	3 20
3	G	226/228~(99%)	208 (92%)	14 (6%)	4 (2%)	8 34
3	Η	226/228~(99%)	205 (91%)	19 (8%)	2(1%)	17 52
3	R	226/228~(99%)	207 (92%)	18 (8%)	1 (0%)	34 69
3	S	226/228~(99%)	201 (89%)	23 (10%)	2(1%)	17 52
3	Т	$22\overline{6}/228~(99\%)$	195 (86%)	24 (11%)	$\overline{7~(3\%)}$	4 23
All	All	4230/4302~(98%)	3758 (89%)	372 (9%)	100 (2%)	6 27

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

5 of 100 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	103	PRO
2	В	201	PHE
2	D	11	LEU
2	Е	191	LYS
3	F	34	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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.



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	160/163~(98%)	132 (82%)	28 (18%)	2	8
1	Q	159/163~(98%)	123 (77%)	36~(23%)	1	3
2	В	277/278~(100%)	264~(95%)	13~(5%)	26	59
2	С	278/278~(100%)	258~(93%)	20 (7%)	14	44
2	D	276/278~(99%)	263~(95%)	13~(5%)	26	59
2	Ε	276/278~(99%)	251 (91%)	25~(9%)	9	33
2	Κ	277/278~(100%)	259 (94%)	18 (6%)	17	47
2	L	278/278~(100%)	260 (94%)	18 (6%)	17	47
2	М	276/278~(99%)	247 (90%)	29 (10%)	7	26
2	Ν	266/278~(96%)	230~(86%)	36 (14%)	4	16
3	F	189/189~(100%)	168 (89%)	21 (11%)	6	24
3	G	189/189~(100%)	178 (94%)	11 (6%)	20	51
3	Н	189/189~(100%)	180 (95%)	9~(5%)	25	58
3	R	189/189~(100%)	178 (94%)	11 (6%)	20	51
3	S	189/189~(100%)	183 (97%)	6 (3%)	39	69
3	Т	189/189~(100%)	182 (96%)	7 (4%)	34	66
All	All	3657/3684 (99%)	3356 (92%)	301 (8%)	11	38

5 of 301 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
2	Ν	214	TYR
3	R	162	ARG
2	Ν	276	VAL
1	Q	114	LEU
3	Т	187	MET

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such side chains are listed below:

Mol	Chain	Res	Type
2	Ν	293	GLN
1	Q	148	ASN
3	R	186	ASN
3	R	153	ASN
3	G	190	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 8 are monoatomic - leaving 14 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	Bos	Link	Bo	Bond lengths		Bond angles		
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
7	ADP	N	401	8	24,29,29	0.95	1 (4%)	29,45,45	1.52	4 (13%)
7	ADP	K	403	8	24,29,29	0.97	1 (4%)	29,45,45	1.48	4 (13%)
7	ADP	М	403	8	24,29,29	0.97	1 (4%)	29,45,45	1.50	4 (13%)
6	AF3	С	402	-	0,3,3	-	-	-		
7	ADP	L	403	8	24,29,29	0.97	1 (4%)	29,45,45	1.44	4 (13%)
6	AF3	K	402	-	0,3,3	-	-	-		
6	AF3	D	402	-	0,3,3	-	-	-		
6	AF3	М	402	-	0,3,3	-	-	-		
6	AF3	L	402	-	0,3,3	-	-	-		
7	ADP	С	403	8	24,29,29	0.96	1 (4%)	29,45,45	1.47	4 (13%)
7	ADP	В	902	8	24,29,29	0.96	1 (4%)	29,45,45	1.56	4 (13%)
7	ADP	Е	401	8	24,29,29	0.97	1 (4%)	29,45,45	1.52	4 (13%)
6	AF3	В	901	-	0,3,3	-	-	-		·
7	ADP	D	403	8	24,29,29	0.96	1 (4%)	29,45,45	1.54	4 (13%)

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
7	ADP	Ν	401	8	-	4/12/32/32	0/3/3/3
7	ADP	K	403	8	-	4/12/32/32	0/3/3/3
7	ADP	М	403	8	-	5/12/32/32	0/3/3/3
7	ADP	L	403	8	-	5/12/32/32	0/3/3/3
7	ADP	С	403	8	-	0/12/32/32	0/3/3/3
7	ADP	В	902	8	-	2/12/32/32	0/3/3/3
7	ADP	Е	401	8	-	4/12/32/32	0/3/3/3
7	ADP	D	403	8	-	0/12/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
7	Κ	403	ADP	C5-C4	2.60	1.47	1.40
7	В	902	ADP	C5-C4	2.56	1.47	1.40
7	Е	401	ADP	C5-C4	2.52	1.47	1.40
7	D	403	ADP	C5-C4	2.51	1.47	1.40
7	Ν	401	ADP	C5-C4	2.51	1.47	1.40

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
7	Е	401	ADP	PA-O3A-PB	-3.93	119.35	132.83
7	В	902	ADP	C3'-C2'-C1'	3.81	106.71	100.98
7	D	403	ADP	PA-O3A-PB	-3.70	120.12	132.83
7	М	403	ADP	C3'-C2'-C1'	3.68	106.52	100.98
7	Κ	403	ADP	C3'-C2'-C1'	3.67	106.50	100.98

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	В	902	ADP	C5'-O5'-PA-O3A
7	Е	401	ADP	C5'-O5'-PA-O1A
7	Е	401	ADP	C5'-O5'-PA-O2A
7	Κ	403	ADP	PA-O3A-PB-O2B
7	Κ	403	ADP	PA-O3A-PB-O3B

There are no ring outliers.



Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	N	401	ADP	5	0
7	K	403	ADP	4	0
7	М	403	ADP	8	0
6	С	402	AF3	1	0
7	L	403	ADP	4	0
6	K	402	AF3	2	0
6	М	402	AF3	3	0
6	L	402	AF3	2	0
7	С	403	ADP	6	0
7	В	902	ADP	8	0
7	Е	401	ADP	6	0
6	В	901	AF3	4	0
7	D	403	ADP	5	0

13 monomers are involved in 53 short contacts:

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

























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 (i)

6.1 Protein, DNA and RNA chains (i)

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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	182/187~(97%)	0.26	13 (7%) 16 6	99, 139, 167, 176	0
1	Q	183/187~(97%)	0.80	34 (18%) 1 0	119, 185, 203, 213	0
2	В	319/320~(99%)	-0.15	0 100 100	59, 89, 109, 139	0
2	С	320/320~(100%)	-0.15	0 100 100	53, 80, 142, 152	0
2	D	318/320~(99%)	-0.14	1 (0%) 94 88	53, 86, 168, 191	0
2	Е	318/320~(99%)	-0.09	6 (1%) 66 46	60, 119, 168, 188	0
2	К	319/320~(99%)	0.15	13 (4%) 37 18	102, 138, 186, 199	0
2	L	320/320~(100%)	0.01	9 (2%) 53 30	89, 116, 197, 206	0
2	М	317/320~(99%)	0.09	9 (2%) 53 30	80, 119, 192, 202	0
2	N	305/320~(95%)	0.41	25 (8%) 11 4	92, 169, 219, 236	0
3	F	228/228~(100%)	0.35	27 (11%) 4 2	110, 144, 189, 213	0
3	G	228/228~(100%)	-0.19	4 (1%) 68 47	75, 105, 128, 151	0
3	Н	228/228~(100%)	0.05	9 (3%) 39 20	92, 125, 172, 180	0
3	R	228/228~(100%)	0.25	19 (8%) 11 4	131, 158, 174, 186	0
3	S	228/228~(100%)	0.18	22 (9%) 8 2	124, 158, 181, 193	0
3	Т	228/228~(100%)	0.40	23 (10%) 7 2	144, 176, 190, 202	0
4	Ι	24/24~(100%)	-0.14	1 (4%) 36 18	80, 160, 248, 304	0
4	Ο	24/24~(100%)	-0.30	0 100 100	106, 187, 271, 291	0
5	J	20/20~(100%)	-0.42	0 100 100	86, 130, 310, 339	0
5	Р	20/20~(100%)	-0.05	3 (15%) 2 1	132, 214, 282, 306	0
All	All	4357/4390 (99%)	0.10	218 (5%) 28 13	53, 131, 192, 339	0

The worst 5 of 218 RSRZ outliers are listed below:



Mol	Chain	Res	Type	RSRZ
1	Q	171	THR	8.5
2	Ν	195	ALA	8.1
1	Q	160	GLY	7.0
3	Т	191	PRO	6.6
1	Q	161	LEU	6.6

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 monosaccharides 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, 95^{th} 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
7	ADP	N	401	27/27	0.86	0.18	148,168,177,180	0
7	ADP	K	403	27/27	0.91	0.26	103,115,122,124	0
7	ADP	Е	401	27/27	0.92	0.18	84,102,106,113	0
7	ADP	D	403	27/27	0.95	0.25	$56,\!66,\!74,\!80$	0
7	ADP	М	403	27/27	0.95	0.27	87,96,107,116	0
7	ADP	В	902	27/27	0.95	0.24	69,71,75,76	0
8	MG	N	402	1/1	0.95	0.55	140,140,140,140	0
7	ADP	L	403	27/27	0.96	0.21	89,97,102,103	0
7	ADP	С	403	27/27	0.96	0.24	54,61,66,67	0
6	AF3	K	402	4/4	0.97	0.35	100,100,101,102	0
6	AF3	В	901	4/4	0.97	0.25	$66,\!67,\!68,\!68$	0
6	AF3	С	402	4/4	0.98	0.23	$54,\!55,\!55,\!55$	0
6	AF3	L	402	4/4	0.98	0.23	85,85,86,87	0
8	MG	В	903	1/1	0.98	0.35	64,64,64,64	0
8	MG	D	401	1/1	0.98	0.35	$59,\!59,\!59,\!59$	0
8	MG	Е	402	1/1	0.98	0.56	79,79,79,79	0
8	MG	K	401	1/1	0.98	0.43	96,96,96,96	0
6	AF3	М	402	4/4	0.98	0.38	83,84,84,85	0
6	AF3	D	402	4/4	0.99	0.28	$5\overline{2},\!56,\!62,\!70$	0

Continued on next page...



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
8	MG	L	401	1/1	0.99	0.23	84,84,84,84	0
8	MG	М	401	1/1	0.99	0.51	84,84,84,84	0
8	MG	С	401	1/1	0.99	0.41	48,48,48,48	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.































6.5 Other polymers (i)

There are no such residues in this entry.

