

wwPDB X-ray Structure Validation Summary Report (i)

Nov 23, 2023 - 12:08 AM JST

PDB ID	:	7X8X
Title	:	structural insights into Mycobacterium tuberculosis ClpP1P2 inhibition by
		Cediranib: implications for developing antimicrobial agents targeting Clp pro-
		tease
Authors	:	Bao, R.; Luo, Y.F.; Zhu, Y.B.; Yang, Y.; Zhou, Y.Z.
Deposited on	:	2022-03-15
Resolution	:	3.24 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 (i)) 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 3.24 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1619 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 chain		
1	А	197	3% 90%	8% •	
1	С	197	88%	11% •	
1	Е	197	3% 93%	5% •	
1	F	197	2% 8 9%	10% ••	I
1	Н	197	91%	8% •	
1	J	197	<mark>6%</mark> 94%	5% ••	I



Mol	Chain	Length	Quality of chain	
1	L	197	5% 97%	6%
		201	5%	0,0 -
1	0	197	93%	6% •
1	Q	197	92%	7% •
1	0	107	9%	
	S	197	96%	••
1	Т	197	96%	• •
1	V	197	10%	6%
-	•	101	6%	070 •
1	Х	197	92%	6% •
1	a	197	91%	7% •
0	D	177	5%	
	D	1//	93% 2%	7%
2	D	177	89%	10% •
2	G	177	92%	7% •
	т	1 7 7	6%	
2	1	177	92%	7% •
2	K	177	94%	5%•
2	М	177	2% 	8%
			4%	0,0 -
2	N	177	94%	5% •
2	Р	177	92%	8%
2	В	177	6%	
	n	111	3%	••
2	U	177	90%	8% •
2	W	177	96%	•••
	N	1 7 7	2%	
2	Y	177	<u>96%</u>	••
2	Z	177	93%	6% •
2	b	177	<u>3%</u> 94%	5% •
	~		33%	370 0
3	0	3	67%	33%
3	1	3	33% 33%	33%
3	2	3	67%	33%



Mol	Chain	Length	Quality of chain						
0	0	0							
3	3	3	67%	33%					
3	4	3	67%	33%					
0	1	0	0770	0,55					
3	с	3	67%	33%					
			33%						
3	е	3	67%	33%					
9	f	9							
0	1	5	67%	33%					
3	g	3	67%	33%					
	0		33%						
3	h	3	67%	33%					
2		9	67%						
3	1	3	67%	33%					
3	i	3	33%	67%					
0	J		0,55	0770					
3	k	3	67%	33%					
_	_		33%						
3	1	3	33% 33%	33%					
3	m	3	220/ 220/	220/					
	111	5	33% 33%	33%					
3	n	3	33% 33%	33%					
			33%						
3	0	3	67%	33%					
9		9	33%						
3	р	3	33%	67%					
3	a	3	67%	33%					
	1		33%						
3	r	3	33% 33%	33%					
		9	33%						
3	S	3	33%	67%					
3	t	3	67%	220/					
0	0	0	0770	0, 55					
3	u	3	67%	33%					
			33%						
3	V	3	33%	67%					
9			33%						
3	W	3	67%	33%					
3	x	3	33%	67%					
3	У	3	33% 33%	33%					
			33%						
3	Z	3	33% 33%	33%					



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	AI4	В	201	-	Х	-	Х
4	AI4	F	301	-	Х	-	Х
4	AI4	G	201	-	Х	-	-
4	AI4	Ι	201	-	Х	-	Х
4	AI4	K	201	-	Х	-	Х
4	AI4	М	201	-	Х	-	-
4	AI4	N	301	-	Х	-	-
4	AI4	R	201	-	Х	-	-
4	AI4	U	201	-	Х	-	Х
4	AI4	V	301	-	Х	-	-
4	AI4	W	201	-	X	-	Х
4	AI4	Y	201	-	Х	-	-
4	AI4	Ζ	201	-	Х	-	-
4	AI4	b	201	-	Х	-	Х

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:



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 81239 atoms, of which 40443 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			Atom	IS			ZeroOcc	AltConf	Trace
1	А	194	Total	С	Н	N	0	S	0	0	0
			2986	936	1495	255	292	8		-	_
1	0	194	Total	С	Н	Ν	0	S	0	0	0
	<u> </u>		2986	936	1495	255	292	8	Ŭ		
1	С	196	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
	0	100	2993	940	1496	256	293	8	0	0	0
1	0	196	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
1	Q	150	2993	940	1496	256	293	8	0	0	0
1	F	106	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
	T,	150	2993	940	1496	256	293	8		0	0
1	1 0	106	Total	С	Η	Ν	0	S	0	0	0
1 5	190	2993	940	1496	256	293	8	0	0	0	
1	тт	196	Total	С	Н	Ν	0	S	0	0	0
	п		3008	943	1507	257	293	8	0	0	0
1	т	196	Total	С	Η	Ν	0	S	0	0	0
	1		3008	943	1507	257	293	8		0	0
1	т	105	Total	С	Н	Ν	0	S	0	0	0
	J	195	3011	946	1509	256	292	8	0	0	
	• •	105	Total	С	Н	Ν	0	S	0	0	0
	V	195	3010	946	1508	256	292	8	0	0	0
	т	100	Total	С	Н	Ν	0	S	0	0	0
	L	193	2941	925	1467	252	289	8	0	0	0
-	37	100	Total	С	Н	N	0	S	0	0	0
	Х	193	2941	925	1467	252	289	8	0	0	0
-		100	Total	С	Н	Ν	0	S	0	0	0
1 E	193	2941	925	1467	252	289	8	0	0	0	
-		100	Total	С	Н	Ν	0	S	0	0	0
	a	193	2941	925	1467	252	289	8	0	0	0

• Molecule 1 is a protein called ATP-dependent Clp protease proteolytic subunit 2.

• Molecule 2 is a protein called ATP-dependent Clp protease proteolytic subunit 1.



Mol	Chain	Residues			Atom	s			ZeroOcc	AltConf	Trace
0	р	177	Total	С	Η	Ν	0	S	0	0	0
	D	111	2695	855	1344	228	259	9	0	0	0
2	р	177	Total	С	Η	Ν	0	S	0	0	0
2	L	111	2695	855	1344	228	259	9	0	0	0
2	Л	175	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
2	D	110	2652	843	1320	223	257	9	0	0	0
2	В	175	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
	10	110	2652	843	1320	223	257	9	0	0	0
2	т	175	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
	-	110	2644	841	1316	223	255	9			0
2	U	175	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
	0	110	2644	841	1316	223	255	9	0	0	0
2	K	175	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
		110	2627	838	1305	220	255	9	Ŭ		0
2	W	175	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
	••		2627	838	1305	220	255	9	0		
2	М	176	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
		110	2629	841	1305	218	256	9	Ŭ		Ŭ
2	Y	176	Total	С	Η	Ν	Ο	S	0	0	0
	-		2629	841	1305	218	256	9	Ŭ		Ű
2	Ν	176	Total	С	Н	N	0	S	0	0	0
			2629	841	1305	218	256	9		_	_
2	Z	176	Total	С	Н	N	0	S	0	0	0
			2629	841	1305	218	256	9		_	_
2	2 G	176	'Total	C	H	N	0	S	0	0	0
		G		2646	844	1316	221	256	9		
2	b	176	'Total	C	H	N	U O	S	0	0	0
		2646	844	1316	221	256	9	-	-	-	

• Molecule 3 is a protein called 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carboxamide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	0	2	Total	С	Η	Ν	0	0	0	0
o c	C	5	52	19	27	2	4	0	0	0
2	0	3	Total	С	Η	Ν	0	0	0	0
o e	е	3	52	19	27	2	4	0		0
2	2 f	3	Total	С	Η	Ν	Ο	0	0	0
J	1		52	19	27	2	4			
9	a.	9	Total	С	Η	Ν	Ο	0	0	0
5 g	g	3	52	19	27	2	4	0		0
2	h	3	Total	С	Η	Ν	Ο	0	0	0
3	11		52	19	27	2	4	0		0



α \cdot \cdot \cdot	C	•	
Continued	trom	premous	naae
contentaca	<i>J</i> · <i>O</i> · · · <i>O</i>	proceeduo	pago

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace	
0		2	Total	С	Н	Ν	0	0	0	0	
3	1	3	52	19	27	2	4	0	0	0	
		2	Total	С	Н	Ν	0	0	6	0	
3	J	3	52	19	27	2	4	0	0	0	
			Total	С	Н	Ν	0				
3 k	3	52	19	27	2	4	0	0	0		
			Total	С	Н	Ν	0				
3	I	3	52	19	27	2	4	0	0	0	
				Total	С	Н	Ν	0			
3	m	3	52	19	27	2	4	0	0	0	
			Total	C	H	Ν	0				
3	n	3	52	19	27	2	4	0	0	0	
			Total C	C	H	N	0				
3	0	3	52	19	27	2	4	0	0	0	
			Total	C	H	N	0				
3	р	3	52	19	27	2	4	0	0	0	
			Total	$\frac{10}{C}$	 	N	$\overline{0}$				
3 q	3	52	19	27	2	Δ	0	0	0		
			Total	$\frac{15}{C}$	<u>-21</u> Н	N	<u>г</u>				
3 r	3	50	10	11 97	2	4	0	0	0		
			J2 Total	$\frac{19}{C}$	 Н	Z N	4				
3	s	3	10tai 59	10	11 97	2	4	0	0	0	
			J2 Total	$\frac{19}{C}$		Z N	$\frac{4}{0}$				
3	t	3	TOTAL 50	10	П 97	11	4	0	0	0	
			02 Total	$\frac{19}{C}$		Z N	4				
3	u	3	Total	10	П 97	IN O	4	0	0	0	
				$\frac{19}{C}$	21	Z	4				
3	v	3	Total	10	H 07	IN O	0	0	0	0	
			52	19	27	2	4				
3	W	3	Total	C	H	N	0	0	0	0	
			52	19	27	2	4				
3	x	3	Total	C	H	N	0	0	0	0	
			52	19	27	2	4				
3	v	3	Total	С	H	N	O	0	0	0	
	7	_	52	19	27	2	4	_	_	_	
3	Z	3	Total	С	Н	Ν	0	0	0	0	
		<u> </u>	52	19	27	2	4	Ŭ	Ŭ	Ŭ	
3	0	3	Total	С	Η	Ν	Ο	0	0	0	
	3 0	3	52	19	27	2	4				
3	3 1	3	Total	\mathbf{C}	Η	Ν	Ο	0	0	0	
3 1	1 J	52	19	27	2	4	U				
2	0	2	Total	С	Η	Ν	Ο	0	0	0	
3		ບ	52	19	27	2	4	0			



MolChainResiduesAtomsZeroOccAltConfT333TotalCHN00J11111111TotalCHN0000TotalCHN000										
Mol	Chain	Residues		\mathbf{At}	\mathbf{oms}			ZeroOcc	AltConf	Trace
2	2	2	Total	С	Η	Ν	Ο	0	0	0
່ <u>ບ</u>	3	5	52	19	27	2	4	0	0	0
2	4	2	Total	С	Η	Ν	Ο	0	0	0
5	4	5	52	19	27	2	4	0	0	0

• Molecule 4 is 4-[1-[3-[4-[(4-fluoranyl-2-methyl-1H-indol-5-yl)oxy]-6-methoxy-quinazolin-7-yl]oxypropyl]piperidin-4-yl]benzamide (three-letter code: AI4) (formula: $C_{33}H_{34}FN_5O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		A	tor	ns			ZeroOcc	AltConf
4	D	1	Total	С	F	Η	Ν	Ο	0	0
4	D	L	71	33	1	28	5	4	0	0
4	D	1	Total	С	F	Η	Ν	Ο	0	0
4 K	L	71	33	1	28	5	4	0	0	
4	Б	1	Total	С	F	Η	Ν	Ο	0	0
4	Г	L	71	33	1	28	5	4	0	0
4	т	1	Total	С	F	Η	Ν	0	0	0
4	1		71	33	1	28	5	4		
4	T	1	Total	С	F	Η	Ν	Ο	0	0
4	U	L	71	33	1	28	5	4	0	
4	V	V 1	Total	С	F	Η	Ν	Ο	0	0
4	v	T	71	33	1	28	5	4	0	0
4	K	1	Total	С	F	Η	Ν	Ο	0	0
4 N	T	71	33	1	28	5	4	0	0	
4	W	1	Total	С	F	Η	Ν	0	0	0
4	vv	L	71	33	1	28	5	4	0	0



Mol	Chain	Residues	-	A	ton	ns			ZeroOcc	AltConf					
4	М	1	Total	С	F	Η	Ν	0	0	0					
4	1/1	1	71	33	1	28	5	4	0	0					
4	V	1	Total	С	F	Η	Ν	0	0	0					
4	1	1	71	33	1	28	5	4	0	0					
4	N	1	Total	С	F	Η	Ν	0	0	0					
4	IN	1	71	33	1	28	5	4							
4	7	7	7	7	7	7	1	Total	С	F	Η	Ν	Ο	0	0
4		1	71	33	1	28	5	4	0	0					
4	С	1	Total	С	F	Η	Ν	Ο	0	0					
4	G	1	71	33	1	28	5	4	0	0					
4	L	1	Total	С	F	Η	Ν	0	0	0					
4	U		71	33	1	28	5	4		U					

Continued from previous page...



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: ATP-dependent Clp protease proteolytic subunit 2



• Molecule 1: ATP-dependent Clp protease proteolytic subunit 2











• Molecule 2: ATP-dependent Clp protease proteolytic subunit 1



5%			
Chain Z:	93%	6% •	
115 117 117 117 118 118 118 118 118 118 118	L104 1120 1120 1130 1135 1135 1135 1135 1135 1135 113	ARG	
• Molecule 2: ATP-o	lependent Clp protease proteo	lytic subunit 1	
Chain G:	92%	7%	
L16 V20 V36 L51 L51 E54 E54 D59	M93 694 694 695 1123 1123 1128 1128 1128 1172 1172 1172 1172 1172		
• Molecule 2: ATP-o	lependent Clp protease proteo	lytic subunit 1	
Chain b:	94%	5%	
L16 V36 E54 M31 E54 M31 C54 C91 C91	M99 L104 L121 M122 H123 H123 H123 H123 H123 H123 M174 A174 A174 A174 A174		
• Molecule 3: 4-[[3,5 amide	-bis(fluoranyl)phenyl]methyl]-	N-[(4-bromophenyl)metl	nyl]piperazine-1-carbo
Chain c:	67%	33%	1
8621 12 13			
• Molecule 3: 4-[[3,5 amide	-bis(fluoranyl)phenyl]methyl]-l	N-[(4-bromophenyl)metl	nyl]piperazine-1-carbo
Chain e:	67%	33%	
• Molecule 3: 4-[[3,5 amide	-bis(fluoranyl)phenyl]methyl]-l	N-[(4-bromophenyl)metl	nyl]piperazine-1-carbo
Chain f:	67%	33%	
BEZ1 L2 L3			
• Molecule 3: 4-[[3,5 amide	-bis(fluoranyl)phenyl]methyl]-l	N-[(4-bromophenyl)metl	nyl]piperazine-1-carbo
Chain g:	67%	33%	



BEZ1 L2 L3

• Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]
methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox amide



 \bullet Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox amide



 \bullet Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox amide

	33%	
Chain j:	33%	67%
.		
E3 E3		

 \bullet Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox amide

Chain k:	67%	33%
BEZ1 L2 L3		

• Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]
methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox amide



• Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]
methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox amide

Chain m:	33%	33%	33%
8621 13 1.3			
			E

• Molecule 3: 4-[[3,5-bis
(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox a
mide



• Molecule 3: 4-[[3,5-bis
(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox a
mide



 \bullet Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox amide

	33%	
Chain p:	33%	67%
BEZ1 L2 L3		

• Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]
methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox amide

Chain q:	e	7%	33%	•
BEZ1 L3 L3				
• Molecule 3 amide	: 4-[[3,5-bis(fluora	nyl)phenyl]methyl]-N	-[(4-bromophenyl)met	hyl]piperazine-1-carbox
Chain r:	33%	220/	2204	
Unam L.	ゴゴ ‰	ゴゴ %	33%	



• Molecule 3: 4-[[3,5-bis
(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox a
mide





• Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]
methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox amide



• Molecule 3: 4-[[3,5-bis
(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox a
mide

Chain u:	67%	33%

• Molecule 3: 4-[[3,5-bis
(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox a
mide

	33%	
Chain v:	33%	67%
.		
BEZ1 L2 L3		

• Molecule 3: 4-[[3,5-bis
(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox a
mide

	33%		
Chain w:	67%	33%	
BEZ1 L2 L3			
 Molecule 	2. 4 [[2.5 big(fluoranyl)nk	onvilmethyll N [(4 bromenhenyl)methy	ullninore

• Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox amide

Chain x:	33%	67%	1
BEZ1 L2 L3			
• Molecul amide	e 3: 4-[[3,5-bis(fluora	nyl)phenyl]methyl]-N-[(4-bromophenyl)meth	nyl]piperazine-1-carbox

α ·			
Chain y:	33%	33%	33%

BEZ1 L2 L3

• Molecule 3: 4-[[3,5-bis
(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox a
mide





• Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]
methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox amide

	33%	
Chain 0:	67%	33%

 \bullet Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox amide

Chain 1:	33%	33%	33%
BEZ1 L2 L3			

67%

• Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]
methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox amide

33%

Chain 2:

BEZ1 L2 L3

BEZ L2 L3

 \bullet Molecule 3: 4-[[3,5-bis(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox amide

α_1 · α_2		
Chain 3:	67%	33%

BEZ1 L2 L3

• Molecule 3: 4-[[3,5-bis
(fluoranyl)phenyl]methyl]-N-[(4-bromophenyl)methyl]piperazine-1-carbox a
mide

Chain 4:	67%	33%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	207.51Å 182.50Å 188.70Å	Depositor
a, b, c, α , β , γ	90.00° 95.02° 90.00°	Depositor
Bosolution(A)	33.31 - 3.24	Depositor
Resolution (A)	136.81 - 3.24	EDS
% Data completeness	99.7(33.31-3.24)	Depositor
(in resolution range)	99.8 (136.81-3.24)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.11 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
D D.	0.179 , 0.254	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.178 , 0.253	DCC
R_{free} test set	5566 reflections (5.02%)	wwPDB-VP
Wilson B-factor $(Å^2)$	98.1	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.39, 58.4	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	81239	wwPDB-VP
Average B, all atoms $(Å^2)$	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 38.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7473e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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: AI4, BEZ

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	B	ond lengths	Bond angles	
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	1.07	5/1512~(0.3%)	1.17	11/2045~(0.5%)
1	С	1.18	12/1518~(0.8%)	1.26	10/2055~(0.5%)
1	Е	1.03	6/1495~(0.4%)	1.09	3/2025~(0.1%)
1	F	1.20	12/1518~(0.8%)	1.29	12/2055~(0.6%)
1	Н	1.16	10/1522~(0.7%)	1.24	10/2059~(0.5%)
1	J	0.94	1/1524~(0.1%)	1.10	7/2062~(0.3%)
1	L	0.94	2/1495~(0.1%)	1.11	8/2025~(0.4%)
1	0	0.93	3/1512~(0.2%)	1.08	7/2045~(0.3%)
1	Q	0.93	2/1518~(0.1%)	1.09	7/2055~(0.3%)
1	S	0.91	2/1518~(0.1%)	1.05	3/2055~(0.1%)
1	Т	1.01	5/1522~(0.3%)	1.07	2/2059~(0.1%)
1	V	0.91	2/1524~(0.1%)	1.12	10/2062~(0.5%)
1	Х	0.97	5/1495~(0.3%)	1.09	7/2025~(0.3%)
1	a	1.03	7/1495~(0.5%)	1.08	5/2025~(0.2%)
2	В	1.03	5/1373~(0.4%)	1.16	10/1856~(0.5%)
2	D	1.10	3/1354~(0.2%)	1.26	13/1831~(0.7%)
2	G	0.98	4/1352~(0.3%)	1.18	10/1830~(0.5%)
2	Ι	1.11	7/1350~(0.5%)	1.24	9/1826~(0.5%)
2	Κ	1.08	6/1344~(0.4%)	1.14	6/1819~(0.3%)
2	М	1.08	5/1346~(0.4%)	1.20	12/1823~(0.7%)
2	Ν	0.94	0/1346	1.19	7/1823~(0.4%)
2	Р	1.01	2/1373~(0.1%)	1.21	10/1856~(0.5%)
2	R	1.04	3/1354~(0.2%)	1.09	3/1831~(0.2%)
2	U	1.05	7/1350~(0.5%)	1.17	6/1826~(0.3%)
2	W	1.02	3/1344~(0.2%)	1.08	3/1819~(0.2%)
2	Y	1.00	2/1346~(0.1%)	1.08	5/1823~(0.3%)
2	Ζ	0.86	1/1346~(0.1%)	1.10	7/1823~(0.4%)
2	b	0.93	3/1352~(0.2%)	1.10	5/1830~(0.3%)
3	0	2.16	1/16~(6.2%)	2.10	0/19
3	1	1.91	0/16	2.97	3/19~(15.8%)
3	2	2.16	1/16~(6.2%)	1.63	0/19
3	3	1.67	0/16	2.14	1/19~(5.3%)



N/-1	Mol Chain		ond lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
3	4	2.16	1/16~(6.2%)	2.87	1/19~(5.3%)	
3	с	1.79	0/16	2.85	1/19~(5.3%)	
3	е	1.91	0/16	1.91	0/19	
3	f	1.88	1/16~(6.2%)	2.47	1/19~(5.3%)	
3	g	2.30	1/16~(6.2%)	3.01	2/19~(10.5%)	
3	h	1.78	0/16	2.96	2/19~(10.5%)	
3	i	2.07	1/16~(6.2%)	2.42	0/19	
3	j	2.15	1/16~(6.2%)	2.53	1/19~(5.3%)	
3	k	2.32	1/16~(6.2%)	2.91	2/19~(10.5%)	
3	1	2.18	1/16~(6.2%)	3.05	2/19~(10.5%)	
3	m	1.81	1/16~(6.2%)	3.00	2/19~(10.5%)	
3	n	1.94	0/16	3.98	3/19~(15.8%)	
3	0	2.49	1/16~(6.2%)	3.65	3/19~(15.8%)	
3	р	2.13	0/16	3.32	4/19~(21.1%)	
3	q	2.62	1/16~(6.2%)	3.50	2/19~(10.5%)	
3	r	1.75	0/16	3.57	4/19~(21.1%)	
3	s	2.18	1/16~(6.2%)	3.27	3/19~(15.8%)	
3	t	2.23	1/16~(6.2%)	2.64	1/19~(5.3%)	
3	u	2.43	1/16~(6.2%)	3.37	3/19~(15.8%)	
3	V	1.90	1/16~(6.2%)	2.66	1/19~(5.3%)	
3	W	2.00	1/16~(6.2%)	2.00	0/19	
3	X	2.06	1/16~(6.2%)	2.17	0/19	
3	У	1.94	1/16~(6.2%)	3.62	2/19~(10.5%)	
3	Z	2.04	0/16	3.88	4/19~(21.1%)	
All	All	1.04	144/40546~(0.4%)	1.18	256/54800~(0.5%)	

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	Ν	0	1
2	Ζ	0	1
All	All	0	2

The worst 5 of 144 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	Q	104	CYS	CB-SG	-10.57	1.64	1.82
1	F	15	ILE	C-N	9.86	1.56	1.34
1	a	151	GLU	CG-CD	9.12	1.65	1.51



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Κ	22	GLU	CG-CD	9.10	1.65	1.51
2	Р	149	GLU	CG-CD	8.69	1.65	1.51

The worst 5 of 256 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	У	2	LEU	O-C-N	-11.09	104.96	122.70
3	Z	3	LEU	CB-CG-CD2	10.51	128.86	111.00
2	K	38	ASP	CB-CG-OD2	-10.39	108.94	118.30
3	0	2	LEU	O-C-N	-10.20	106.38	122.70
3	n	3	LEU	CB-CG-CD2	9.92	127.86	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Ν	18	ASP	Peptide
2	Ζ	18	ASP	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	Perce	ntiles
1	А	192/197~(98%)	183 (95%)	8 (4%)	1 (0%)	29	64
1	С	194/197~(98%)	186 (96%)	7 (4%)	1 (0%)	29	64
1	Е	191/197~(97%)	180 (94%)	11 (6%)	0	100	100
1	F	194/197~(98%)	185 (95%)	7 (4%)	2 (1%)	15	50



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Continucu	110116	$p_{1}c_{0}a_{0}a_{0}$	page
	9	1	1 0

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	Н	194/197~(98%)	184 (95%)	10 (5%)	0	100	100
1	J	193/197~(98%)	182 (94%)	11 (6%)	0	100	100
1	L	191/197~(97%)	183 (96%)	8 (4%)	0	100	100
1	Ο	192/197~(98%)	181 (94%)	10 (5%)	1 (0%)	29	64
1	Q	194/197~(98%)	186 (96%)	7 (4%)	1 (0%)	29	64
1	S	194/197~(98%)	183 (94%)	10 (5%)	1 (0%)	29	64
1	Т	194/197~(98%)	188 (97%)	6 (3%)	0	100	100
1	V	193/197~(98%)	182 (94%)	10 (5%)	1 (0%)	29	64
1	Х	191/197~(97%)	181 (95%)	9(5%)	1 (0%)	29	64
1	a	191/197~(97%)	182 (95%)	9(5%)	0	100	100
2	В	175/177~(99%)	168 (96%)	7 (4%)	0	100	100
2	D	173/177~(98%)	168 (97%)	5 (3%)	0	100	100
2	G	174/177~(98%)	169 (97%)	5 (3%)	0	100	100
2	Ι	173/177~(98%)	170 (98%)	2 (1%)	1 (1%)	25	61
2	К	173/177~(98%)	166 (96%)	7 (4%)	0	100	100
2	М	174/177~(98%)	169 (97%)	4 (2%)	1 (1%)	25	61
2	Ν	174/177~(98%)	169 (97%)	5 (3%)	0	100	100
2	Р	175/177~(99%)	169 (97%)	5 (3%)	1 (1%)	25	61
2	R	173/177~(98%)	168 (97%)	5 (3%)	0	100	100
2	U	173/177~(98%)	169 (98%)	3 (2%)	1 (1%)	25	61
2	W	173/177~(98%)	167 (96%)	6 (4%)	0	100	100
2	Y	174/177~(98%)	169 (97%)	5 (3%)	0	100	100
2	Ζ	174/177~(98%)	167 (96%)	7 (4%)	0	100	100
2	b	174/177~(98%)	168 (97%)	5 (3%)	1 (1%)	25	61
3	0	1/3~(33%)	1 (100%)	0	0	100	100
3	1	1/3~(33%)	1 (100%)	0	0	100	100
3	2	1/3~(33%)	1 (100%)	0	0	100	100
3	3	1/3~(33%)	1 (100%)	0	0	100	100
3	4	1/3~(33%)	1 (100%)	0	0	100	100
3	с	1/3~(33%)	1 (100%)	0	0	100	100
3	e	1/3~(33%)	1 (100%)	0	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
3	f	1/3~(33%)	1 (100%)	0	0	100	100
3	g	1/3~(33%)	1 (100%)	0	0	100	100
3	h	1/3~(33%)	1 (100%)	0	0	100	100
3	i	1/3~(33%)	0	1 (100%)	0	100	100
3	j	1/3~(33%)	1 (100%)	0	0	100	100
3	k	1/3~(33%)	1 (100%)	0	0	100	100
3	1	1/3~(33%)	1 (100%)	0	0	100	100
3	m	1/3~(33%)	0	0	1 (100%)	0	0
3	n	1/3~(33%)	1 (100%)	0	0	100	100
3	О	1/3~(33%)	1 (100%)	0	0	100	100
3	р	1/3~(33%)	1 (100%)	0	0	100	100
3	q	1/3~(33%)	0	1 (100%)	0	100	100
3	r	1/3~(33%)	1 (100%)	0	0	100	100
3	S	1/3~(33%)	0	1 (100%)	0	100	100
3	t	1/3~(33%)	1 (100%)	0	0	100	100
3	u	1/3~(33%)	1 (100%)	0	0	100	100
3	v	1/3~(33%)	1 (100%)	0	0	100	100
3	W	1/3~(33%)	1 (100%)	0	0	100	100
3	х	1/3~(33%)	1 (100%)	0	0	100	100
3	У	1/3~(33%)	1 (100%)	0	0	100	100
3	Z	1/3~(33%)	1 (100%)	0	0	100	100
All	All	5158/5320 (97%)	4946 (96%)	197 (4%)	15 (0%)	41	73

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Р	94	GLY
2	U	94	GLY
1	V	106	GLY
2	b	94	GLY
3	m	2	LEU



5.3.2 Protein sidechains (i)

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	А	160/164~(98%)	159~(99%)	1 (1%)	86	93
1	\mathbf{C}	160/164~(98%)	158~(99%)	2(1%)	69	85
1	Ε	157/164~(96%)	155~(99%)	2(1%)	69	85
1	F	160/164~(98%)	159~(99%)	1 (1%)	86	93
1	Η	161/164~(98%)	161 (100%)	0	100	100
1	J	161/164~(98%)	158 (98%)	3 (2%)	57	79
1	L	157/164~(96%)	155 (99%)	2 (1%)	69	85
1	Ο	160/164~(98%)	160 (100%)	0	100	100
1	Q	160/164~(98%)	157 (98%)	3 (2%)	57	79
1	S	160/164~(98%)	159 (99%)	1 (1%)	86	93
1	Т	161/164~(98%)	161 (100%)	0	100	100
1	V	161/164~(98%)	160 (99%)	1 (1%)	86	93
1	Х	157/164~(96%)	157 (100%)	0	100	100
1	a	157/164~(96%)	153 (98%)	4 (2%)	47	74
2	В	138/138 (100%)	138 (100%)	0	100	100
2	D	136/138~(99%)	134 (98%)	2(2%)	65	83
2	G	135/138~(98%)	134 (99%)	1 (1%)	84	92
2	Ι	135/138~(98%)	134 (99%)	1 (1%)	84	92
2	К	134/138~(97%)	134 (100%)	0	100	100
2	М	134/138~(97%)	132 (98%)	2(2%)	65	83
2	Ν	134/138~(97%)	132 (98%)	2(2%)	65	83
2	Р	$1\overline{38/138}~(100\%)$	137 (99%)	1 (1%)	84	92
2	R	136/138~(99%)	134 (98%)	2(2%)	65	83
2	U	$13\overline{5}/138~(98\%)$	134 (99%)	1 (1%)	84	92
2	W	134/138~(97%)	134 (100%)	0	100	100
2	Y	$\overline{134/138}\ (97\%)$	133 (99%)	1 (1%)	84	92



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contentaca	<i>J</i> · <i>O</i> · · · <i>O</i>	proceed ac	pagem

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
2	Ζ	134/138~(97%)	132 (98%)	2(2%)	65	83
2	b	135/138~(98%)	134 (99%)	1 (1%)	84	92
3	0	2/2~(100%)	1 (50%)	1 (50%)	0	0
3	1	2/2~(100%)	1 (50%)	1 (50%)	0	0
3	2	2/2~(100%)	2 (100%)	0	100	100
3	3	2/2~(100%)	1 (50%)	1 (50%)	0	0
3	4	2/2~(100%)	1 (50%)	1 (50%)	0	0
3	с	2/2~(100%)	2 (100%)	0	100	100
3	е	2/2~(100%)	1 (50%)	1 (50%)	0	0
3	f	2/2~(100%)	2 (100%)	0	100	100
3	g	2/2~(100%)	2 (100%)	0	100	100
3	h	2/2~(100%)	1 (50%)	1 (50%)	0	0
3	i	2/2~(100%)	2 (100%)	0	100	100
3	j	2/2~(100%)	1 (50%)	1 (50%)	0	0
3	k	2/2~(100%)	1 (50%)	1 (50%)	0	0
3	1	2/2~(100%)	1 (50%)	1 (50%)	0	0
3	m	2/2~(100%)	0	2 (100%)	0	0
3	n	2/2~(100%)	1 (50%)	1 (50%)	0	0
3	О	2/2~(100%)	1 (50%)	1 (50%)	0	0
3	р	2/2~(100%)	0	2 (100%)	0	0
3	q	2/2~(100%)	1 (50%)	1 (50%)	0	0
3	r	2/2~(100%)	1 (50%)	1 (50%)	0	0
3	s	2/2~(100%)	2(100%)	0	100	100
3	t	2/2~(100%)	2(100%)	0	100	100
3	u	2/2~(100%)	2(100%)	0	100	100
3	V	2/2~(100%)	0	2 (100%)	0	0
3	W	2/2~(100%)	2 (100%)	0	100	100
3	х	2/2~(100%)	1 (50%)	1 (50%)	0	0
3	У	2/2~(100%)	0	2 (100%)	0	0
3	Z	2/2~(100%)	0	2 (100%)	0	0
All	All	4180/4284 (98%)	4120 (99%)	60 (1%)	67	84



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5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	\mathbf{Type}
1	Ε	87	MET
3	Z	3	LEU
2	b	123	HIS
3	Z	2	LEU
3	4	2	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	Н	94	GLN
1	L	94	GLN
2	G	47	GLN
1	L	135	HIS
1	Q	135	HIS

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)

14 ligands are modelled in this entry.

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).



Mal	Mol Type Chair		Bos	Tink	В	ond leng	gths	B	ond ang	gles
	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AI4	К	201	-	45,48,48	<mark>5.54</mark>	24 (53%)	62,68,68	4.95	32 (51%)
4	AI4	Y	201	-	45,48,48	5.64	24 (53%)	62,68,68	5.17	32 (51%)
4	AI4	U	201	-	45,48,48	5.46	26 (57%)	62,68,68	5.10	33 (53%)
4	AI4	Ι	201	-	45,48,48	5.56	27 (60%)	62,68,68	5.05	33 (53%)
4	AI4	Z	201	-	45,48,48	<mark>5.68</mark>	26 (57%)	62,68,68	5.13	32 (51%)
4	AI4	W	201	-	45,48,48	5.61	28 (62%)	62,68,68	4.39	32 (51%)
4	AI4	G	201	-	45,48,48	<mark>5.60</mark>	27 (60%)	62,68,68	5.07	37 (59%)
4	AI4	F	301	-	45,48,48	5.62	26 (57%)	62,68,68	4.81	31 (50%)
4	AI4	Ν	301	-	45,48,48	5.62	21 (46%)	62,68,68	8.67	39 (62%)
4	AI4	В	201	-	45,48,48	5.47	24 (53%)	62,68,68	5.51	38 (61%)
4	AI4	b	201	-	45,48,48	5.60	24 (53%)	62,68,68	5.15	37 (59%)
4	AI4	V	301	-	45,48,48	5.60	26 (57%)	62,68,68	4.89	33 (53%)
4	AI4	М	201	-	45,48,48	<mark>5.59</mark>	25 (55%)	62,68,68	4.79	35 (56%)
4	AI4	R	201	-	45,48,48	5.52	22 (48%)	62,68,68	4.76	34 (54%)

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
4	AI4	К	201	-	-	10/21/31/31	0/6/6/6
4	AI4	Y	201	-	-	11/21/31/31	0/6/6/6
4	AI4	U	201	-	-	12/21/31/31	0/6/6/6
4	AI4	Ι	201	-	-	10/21/31/31	0/6/6/6
4	AI4	Z	201	-	-	11/21/31/31	0/6/6/6
4	AI4	W	201	-	-	9/21/31/31	0/6/6/6
4	AI4	G	201	-	-	11/21/31/31	0/6/6/6
4	AI4	F	301	-	-	9/21/31/31	0/6/6/6
4	AI4	Ν	301	-	-	10/21/31/31	0/6/6/6
4	AI4	В	201	-	-	10/21/31/31	0/6/6/6
4	AI4	b	201	-	-	10/21/31/31	0/6/6/6
4	AI4	V	301	-	-	10/21/31/31	0/6/6/6
4	AI4	М	201	-	-	13/21/31/31	0/6/6/6
4	AI4	R	201	-	-	11/21/31/31	0/6/6/6



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	301	AI4	C36-C35	-16.96	1.11	1.39
4	Ι	201	AI4	C40-C35	-16.94	1.11	1.39
4	b	201	AI4	C40-C35	-16.94	1.11	1.39
4	R	201	AI4	C40-C35	-16.85	1.11	1.39
4	Ν	301	AI4	C36-C35	-16.67	1.12	1.39

The worst 5 of 350 bond length outliers are listed below:

The worst 5 of 478 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	N	301	AI4	O43-C41-N42	-41.95	62.98	122.58
4	N	301	AI4	O43-C41-C38	-36.76	75.64	119.63
4	Y	201	AI4	C38-C41-N42	18.11	139.48	117.75
4	N	301	AI4	C38-C41-N42	17.39	138.62	117.75
4	В	201	AI4	O43-C41-N42	-16.43	99.24	122.58

There are no chirality outliers.

5 of 147 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	U	201	AI4	C15-C14-O13-C10
4	Κ	201	AI4	C15-C14-O13-C10
4	М	201	AI4	C15-C14-O13-C10
4	b	201	AI4	C15-C14-O13-C10
4	W	201	AI4	C26-C27-N28-C30

There are no ring outliers.

No monomer is involved in 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, 95^{th} 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		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	194/197~(98%)	0.58	5 (2%) 56 4	4	64,87,119,144	0
1	\mathbf{C}	196/197~(99%)	0.64	8 (4%) 37 2	27	57, 82, 115, 155	0
1	Ε	193/197~(97%)	0.59	6 (3%) 49 3	87	69, 90, 121, 137	0
1	F	196/197~(99%)	0.61	3 (1%) 73 6	54	65, 83, 113, 175	0
1	Н	196/197~(99%)	0.61	8 (4%) 37 2	27	63,81,125,174	0
1	J	195/197~(98%)	0.63	11 (5%) 24	15	75, 96, 125, 154	0
1	L	193/197~(97%)	0.68	9 (4%) 31 2	21	75, 97, 121, 142	0
1	Ο	194/197~(98%)	0.63	10 (5%) 27	17	79, 97, 134, 154	0
1	Q	196/197~(99%)	0.69	14 (7%) 16	11	77, 102, 133, 157	0
1	S	196/197~(99%)	0.75	17 (8%) 10	7	76,105,139,173	0
1	Т	196/197~(99%)	0.72	13 (6%) 18	12	77, 97, 132, 190	0
1	V	195/197~(98%)	0.74	19 (9%) 7	6	78, 100, 135, 166	0
1	Х	193/197~(97%)	0.75	12 (6%) 20	13	79, 102, 130, 147	0
1	a	193/197~(97%)	0.66	12 (6%) 20	13	74, 97, 126, 142	0
2	В	177/177~(100%)	0.62	8 (4%) 33 2	23	65, 87, 123, 149	0
2	D	175/177~(98%)	0.55	4 (2%) 60 5	50	64, 83, 116, 139	0
2	G	176/177~(99%)	0.58	4 (2%) 60 5	50	66, 87, 119, 145	0
2	Ι	175/177~(98%)	0.61	11 (6%) 20	13	66, 81, 111, 143	0
2	Κ	175/177~(98%)	0.70	17 (9%) 7	6	71, 93, 122, 148	0
2	М	176/177~(99%)	0.59	3 (1%) 70 6	50	64, 82, 109, 132	0
2	Ν	176/177~(99%)	0.64	7(3%) 38 2	28	67, 90, 125, 156	0
2	Р	$1\overline{77/177~(100\%)}$	0.58	6 (3%) 45 3	3	$6\overline{8}, 89, 117, 142$	0
2	R	175/177~(98%)	0.66	10 (5%) 23	15	71, 90, 120, 148	0
2	U	$17\overline{5/177}~(98\%)$	0.59	6(3%) 45 3	33	72, 87, 112, 132	0



Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
2	W	175/177~(98%)	0.66	8 (4%) 32 22	73, 92, 124, 142	0
2	Y	176/177~(99%)	0.60	4 (2%) 60 50	69,88,115,146	0
2	Z	176/177~(99%)	0.68	8 (4%) 33 23	72, 95, 125, 157	0
2	b	176/177~(99%)	0.60	6 (3%) 45 33	73, 91, 117, 145	0
3	0	2/3~(66%)	1.68	1 (50%) 0 0	123, 123, 123, 128	0
3	1	2/3~(66%)	1.34	0 100 100	103, 103, 103, 111	0
3	2	2/3~(66%)	0.82	0 100 100	125, 125, 125, 125	0
3	3	2/3~(66%)	1.51	0 100 100	104, 104, 104, 106	0
3	4	2/3~(66%)	0.48	0 100 100	126, 126, 126, 132	0
3	с	2/3~(66%)	1.70	0 100 100	104, 104, 104, 106	0
3	е	2/3~(66%)	1.65	1 (50%) 0 0	115, 115, 115, 125	0
3	f	2/3~(66%)	1.43	0 100 100	97, 97, 97, 97, 97	0
3	g	2/3~(66%)	1.26	0 100 100	123, 123, 123, 133	0
3	h	2/3~(66%)	2.07	1 (50%) 0 0	92, 92, 92, 103	0
3	i	2/3~(66%)	2.65	2 (100%) 0 0	113, 113, 113, 119	0
3	j	2/3~(66%)	2.74	1 (50%) 0 0	90, 90, 90, 100	0
3	k	2/3~(66%)	1.16	0 100 100	115, 115, 115, 126	0
3	1	2/3~(66%)	2.81	1 (50%) 0 0	94, 94, 94, 110	0
3	m	2/3~(66%)	0.81	0 100 100	116, 116, 116, 120	0
3	n	2/3~(66%)	1.79	1 (50%) 0 0	100, 100, 100, 104	0
3	0	2/3~(66%)	2.66	1 (50%) 0 0	120, 120, 120, 121	0
3	р	2/3~(66%)	3.17	1 (50%) 0 0	94, 94, 94, 105	0
3	q	2/3~(66%)	0.66	0 100 100	127, 127, 127, 130	0
3	r	2/3~(66%)	1.55	1 (50%) 0 0	97, 97, 97, 100	0
3	S	2/3~(66%)	2.44	1 (50%) 0 0	119, 119, 119, 126	0
3	t	2/3~(66%)	2.11	1 (50%) 0 0	99, 99, 99, 107	0
3	u	2/3~(66%)	1.36	0 100 100	119, 119, 119, 128	0
3	V	2/3~(66%)	2.39	1 (50%) 0 0	96, 96, 96, 105	0
3	W	2/3~(66%)	1.39	1 (50%) 0 0	121, 121, 121, 126	0
3	X	2/3~(66%)	1.71	0 100 100	$1\overline{03, 103, 103, 103, 107}$	0
3	у	2/3~(66%)	0.71	0 100 100	128, 128, 128, 137	0



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Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2		$\cdot 2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	$Q{<}0.9$
3	Z	2/3~(66%)	1.50	1 (50%)	0	0	99, 99, 99, 101	0
All	All	5242/5320~(98%)	0.65	265~(5%)	28	18	57, 92, 125, 190	0

The worst 5 of 265 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Т	210	SER	8.8
1	S	210	SER	6.2
1	Т	209	LEU	6.1
3	р	3	LEU	4.9
3	s	3	LEU	4.9

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
4	AI4	W	201	43/43	0.64	0.56	111,157,195,219	0
4	AI4	U	201	43/43	0.70	0.55	103,148,191,204	0
4	AI4	K	201	43/43	0.77	0.49	114,146,188,204	0
4	AI4	В	201	43/43	0.77	0.52	105,138,204,223	0
4	AI4	b	201	43/43	0.77	0.47	107,140,184,201	0
4	AI4	Ι	201	43/43	0.78	0.44	104,137,196,215	0
4	AI4	F	301	43/43	0.79	0.47	96,133,190,200	0
4	AI4	G	201	43/43	0.80	0.58	100,137,201,215	0
4	AI4	V	301	43/43	0.81	0.45	101,135,192,215	0
4	AI4	Z	201	43/43	0.84	0.51	99,149,213,226	0
4	AI4	М	201	43/43	0.84	0.42	99,135,199,215	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9			
4	AI4	Y	201	43/43	0.84	0.58	102, 136, 195, 209	0			
4	AI4	R	201	43/43	0.85	0.48	94,136,203,221	0			
4	AI4	N	301	43/43	0.86	0.42	90,134,190,200	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.

