

wwPDB X-ray Structure Validation Summary Report (i)

Mar 3, 2024 - 08:06 PM EST

PDB ID	:	$6\mathrm{EE2}$
Title	:	X-ray crystal structure of Pf-M17 in complex with inhibitor 6i and regulatory
		zinc ion
Authors	:	Drinkwater, N.; McGowan, S.
Deposited on	:	2018-08-13
Resolution	:	2.10 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 2.10 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.



Motrie	Whole archive	Similar resolution		
WIEUTIC	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R_{free}	130704	5197 (2.10-2.10)		
Clashscore	141614	5710 (2.10-2.10)		
Ramachandran outliers	138981	5647 (2.10-2.10)		
Sidechain outliers	138945	5648 (2.10-2.10)		
RSRZ outliers	127900	5083 (2.10-2.10)		

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 chain	
1	А	526	91%	7% •
1	В	526	% 90%	8% •
1	С	526	92%	6% •
1	D	526	91%	6% ·
1	Е	526	87%	10% •



Conti	Continuea from previous page						
Mol	Chain	Length	Quality of chain				
1	F	526	89%	7% •			
1	G	526	90%	8% ••			
1	Н	526	2% 91%	7% •			
1	Ι	526	% • 94%	6% ·			
1	J	526	90%	7% •			
1	Κ	526	87%	9% •			
1	L	526	90%	8% •			

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	1PE	L	709	-	-	Х	-



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 52312 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	Δ	510	Total	С	Ν	0	S	0	1	0
1	A	519	3994	2563	642	769	20	0	1	0
1	р	519	Total	С	Ν	0	S	0	1	0
1	D	510	3952	2541	642	749	20	0	1	0
1	C	520	Total	С	Ν	0	S	0	1	0
1		520	3994	2567	643	764	20	0	1	0
1	П	516	Total	С	Ν	0	S	0	2	0
1	D	510	3955	2549	639	746	21	0	2	0
1	F	510	Total	С	Ν	0	S	0	0	0
1		510	3912	2516	631	746	19	0		
1	Б	510	Total	С	Ν	0	S	0	1	0
1	Г	510	3890	2502	627	742	19	0	T	0
1	C	510	Total	С	Ν	0	S	0	1	0
1	G	519	3993	2563	645	765	20	0	1	0
1	и	500	Total	С	Ν	0	S	0	1	0
1	11	520	3960	2548	640	752	20	0	1	U
1	т	502	Total	С	Ν	0	S	0	0	0
1	1	525	3992	2561	644	767	20	0	0	0
1	т	519	Total	С	Ν	0	S	0	0	0
1	J	512	3927	2528	636	743	20	0	0	0
1	K	500	Total	С	Ν	0	S	0	0	0
	IX	509	3900	2511	627	743	19	U		U
1	т	513	Total	С	Ν	0	S	0	0	0
		515	3910	2511	632	748	19	U	U	U

• Molecule 1 is a protein called Pf-M17.

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	152	GLN	ASN	engineered mutation	UNP W4I9J7
А	515	GLN	ASN	engineered mutation	UNP W4I9J7
А	546	GLN	ASN	engineered mutation	UNP W4I9J7
А	606	HIS	-	expression tag	UNP W4I9J7
А	607	HIS	-	expression tag	UNP W4I9J7



А

А

А

Comment

expression tag

Actual

_

HIS	-	expression tag	UNP W4I9J7
HIS	-	expression tag	UNP W4I9J7
GLN	ASN	engineered mutation	UNP W4I9J7
GLN	ASN	engineered mutation	UNP W4I9J7
GLN	ASN	engineered mutation	UNP W4I9J7
HIS	-	expression tag	UNP W4I9J7
HIS	-	expression tag	UNP W4I9J7
HIS	-	expression tag	UNP W4I9J7
HIS	-	expression tag	UNP W4I9J7
HIS	-	expression tag	UNP W4I9J7
GLN	ASN	engineered mutation	UNP W4I9J7
GLN	ASN	engineered mutation	UNP W4I9J7
GLN	ASN	engineered mutation	UNP W4I9J7
HIS	-	expression tag	UNP W4I9J7
HIS	-	expression tag	UNP W4I9J7
HIS	-	expression tag	UNP W4I9J7
HIS	-	expression tag	UNP W4I9J7
HIS	-	expression tag	UNP W4I9J7
GLN	ASN	engineered mutation	UNP W4I9J7
GLN	ASN	engineered mutation	UNP W4I9J7
GLN	ASN	engineered mutation	UNP W4I9J7
HIS	-	expression tag	UNP W4I9J7
HIS	-	expression tag	UNP W4I9J7
HIS	-	expression tag	UNP W4I9J7
HIS	-	expression tag	UNP W4I9J7

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HIS

608

609

610

В	152	GLN	ASN	engineered mutation	UNP W4I9J7
В	515	GLN	ASN	engineered mutation	UNP W4I9J7
В	546	GLN	ASN	engineered mutation	UNP W4I9J7
В	606	HIS	-	expression tag	UNP W4I9J7
В	607	HIS	-	expression tag	UNP W4I9J7
В	608	HIS	-	expression tag	UNP W4I9J7
В	609	HIS	-	expression tag	UNP W4I9J7
В	610	HIS	-	expression tag	UNP W4I9J7
С	152	GLN	ASN	engineered mutation	UNP W4I9J7
С	515	GLN	ASN	engineered mutation	UNP W4I9J7
С	546	GLN	ASN	engineered mutation	UNP W4I9J7
С	606	HIS	-	expression tag	UNP W4I9J7
С	607	HIS	-	expression tag	UNP W4I9J7
С	608	HIS	-	expression tag	UNP W4I9J7
С	609	HIS	-	expression tag	UNP W4I9J7
С	610	HIS	-	expression tag	UNP W4I9J7
D	152	GLN	ASN	engineered mutation	UNP W4I9J7
D	515	GLN	ASN	engineered mutation	UNP W4I9J7
D	546	GLN	ASN	engineered mutation	UNP W4I9J7
D	606	HIS	-	expression tag	UNP W4I9J7
D	607	HIS	-	expression tag	UNP W4I9J7
D	608	HIS	-	expression tag	UNP W4I9J7
D	609	HIS	-	expression tag	UNP W4I9J7
D	610	HIS	-	expression tag	UNP W4I9J7
E	152	GLN	ASN	engineered mutation	UNP W4I9J7
E	515	GLN	ASN	engineered mutation	UNP W4I9J7
E	546	GLN	ASN	engineered mutation	UNP W4I9J7
Е	606	HIS	-	expression tag	UNP W4I9J7
Е	607	HIS	-	expression tag	UNP W4I9J7
Е	608	HIS	-	expression tag	UNP W4I9J7
E	609	HIS	-	expression tag	UNP W4I9J7
Е	610	HIS	-	expression tag	UNP W4I9J7
F	152	GLN	ASN	engineered mutation	UNP W4I9J7
F	515	GLN	ASN	engineered mutation	UNP W4I9J7
F	546	GLN	ASN	engineered mutation	UNP W4I9J7
F	606	HIS	-	expression tag	UNP W4I9J7
F	607	HIS	-	expression tag	UNP W4I9J7
F	608	HIS	-	expression tag	UNP W4I9J7
F	609	HIS	-	expression tag	UNP W4I9J7
				0 1: 1	

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Reference

UNP W4I9J7



Chain	Residue	Modelled	Actual	Comment	Reference
F	610	HIS	-	expression tag	UNP W4I9J7
G	152	GLN	ASN	engineered mutation	UNP W4I9J7
G	515	GLN	ASN	engineered mutation	UNP W4I9J7
G	546	GLN	ASN	engineered mutation	UNP W4I9J7
G	606	HIS	-	expression tag	UNP W4I9J7
G	607	HIS	-	expression tag	UNP W4I9J7
G	608	HIS	-	expression tag	UNP W4I9J7
G	609	HIS	-	expression tag	UNP W4I9J7
G	610	HIS	-	expression tag	UNP W4I9J7
Н	152	GLN	ASN	engineered mutation	UNP W4I9J7
Н	515	GLN	ASN	engineered mutation	UNP W4I9J7
Н	546	GLN	ASN	engineered mutation	UNP W4I9J7
Н	606	HIS	-	expression tag	UNP W4I9J7
Н	607	HIS	-	expression tag	UNP W4I9J7
Н	608	HIS	-	expression tag	UNP W4I9J7
Н	609	HIS	-	expression tag	UNP W4I9J7
Н	610	HIS	-	expression tag	UNP W4I9J7
Ι	152	GLN	ASN	engineered mutation	UNP W4I9J7
Ι	515	GLN	ASN	engineered mutation	UNP W4I9J7
Ι	546	GLN	ASN	engineered mutation	UNP W4I9J7
Ι	606	HIS	-	expression tag	UNP W4I9J7
Ι	607	HIS	-	expression tag	UNP W4I9J7
Ι	608	HIS	-	expression tag	UNP W4I9J7
Ι	609	HIS	-	expression tag	UNP W4I9J7
Ι	610	HIS	-	expression tag	UNP W4I9J7
J	152	GLN	ASN	engineered mutation	UNP W4I9J7
J	515	GLN	ASN	engineered mutation	UNP W4I9J7
J	546	GLN	ASN	engineered mutation	UNP W4I9J7
J	606	HIS	-	expression tag	UNP W4I9J7
J	607	HIS	-	expression tag	UNP W4I9J7
J	608	HIS	-	expression tag	UNP W4I9J7
J	609	HIS	-	expression tag	UNP W4I9J7
J	610	HIS	-	expression tag	UNP W4I9J7
K	152	GLN	ASN	engineered mutation	UNP W4I9J7
K	515	GLN	ASN	engineered mutation	UNP W4I9J7
K	546	GLN	ASN	engineered mutation	UNP W4I9J7
K	606	HIS	-	expression tag	UNP W4I9J7
K	607	HIS	-	expression tag	UNP W4I9J7
K	608	HIS	-	expression tag	UNP W4I9J7
K	609	HIS	-	expression tag	UNP W4I9J7
K	610	HIS	-	expression tag	UNP W4I9J7
L	152	GLN	ASN	engineered mutation	UNP W4I9J7

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Chain	Residue	Modelled	Actual	Comment	Reference
L	515	GLN	ASN	engineered mutation	UNP W4I9J7
L	546	GLN	ASN	engineered mutation	UNP W4I9J7
L	606	HIS	-	expression tag	UNP W4I9J7
L	607	HIS	-	expression tag	UNP W4I9J7
L	608	HIS	-	expression tag	UNP W4I9J7
L	609	HIS	-	expression tag	UNP W4I9J7
L	610	HIS	-	expression tag	UNP W4I9J7

• Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 1 & 3 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 1 & 3 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 1 & 3 \end{array}$	0	0
2	D	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 1 3 \end{array}$	0	0
2	Ε	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 1 & 3 \end{array}$	0	0
2	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 1 & 3 \end{array}$	0	0
2	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 1 & 3 \end{array}$	0	0
2	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 1 & 3 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 1 & 3 \end{array}$	0	0
2	J	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 1 & 3 \end{array}$	0	0
2	Κ	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 1 3 \end{array}$	0	0
2	L	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 1 3 \end{array}$	0	0

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Zn 1 1	0	0
3	В	1	Total Zn 1 1	0	0
3	С	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	Е	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0
3	G	1	Total Zn 1 1	0	0
3	Н	1	Total Zn 1 1	0	0
3	Ι	1	Total Zn 1 1	0	0
3	J	1	Total Zn 1 1	0	0
3	К	1	Total Zn 1 1	0	0
3	L	1	Total Zn 1 1	0	0

• Molecule 4 is N-[(1R)-2-(hydroxyamino)-2-oxo-1-(3',4',5'-trifluoro[1,1'-biphenyl]-4-yl)eth yl]cyclohexanecarboxamide (three-letter code: J1V) (formula: $C_{21}H_{21}F_3N_2O_3$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
4	٨	1	Total	С	F	Ν	Ο	0	0
4	A	L	29	21	3	2	3	0	0
4	D	1	Total	С	F	Ν	0	0	0
4	D	L	29	21	3	2	3	0	0
4	С	1	Total	С	F	Ν	0	0	0
4	U	T	29	21	3	2	3	0	0
4	Л	1	Total	С	F	Ν	Ο	0	0
4	D	T	29	21	3	2	3	0	0
4	F	1	Total	С	F	Ν	Ο	0	0
4	Ľ	T	29	21	3	2	3	0	0
4	F	1	Total	С	\mathbf{F}	Ν	Ο	0	0
	1		29	21	3	2	3		0
4	G	1	Total	\mathbf{C}	F	Ν	Ο	0	0
1		1	29	21	3	2	3	0	0
4	Н	1	Total	С	F	Ν	Ο	0	0
-	11	1	29	21	3	2	3	0	0
4	Т	1	Total	С	F	Ν	Ο	0	0
-	1	1	29	21	3	2	3	0	0
4	Т	1	Total	С	F	Ν	Ο	0	0
		T	29	21	3	2	3	0	0
4	K	1	Total	\mathbf{C}	F	Ν	Ο	0	0
	11		29	21	3	2	3	0	0
4	L	1	Total	С	F	Ν	Ο	0	0
Т			29	21	3	2	3		

• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	Е	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	G	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
5	G	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total O S	0	0
0	<u> </u>	1	5 4 1	0	0
5	T	1	Total O S	0	0
	-	-	5 4 1		
5	Ι	1	Total O S	0	0
	-	-	5 4 1	Ŭ	0
5	Κ	1	Total O S	0	0
			5 4 1		_
5	Κ	1	Total O S	0	0
			<u>5 4 1</u>		
5	Κ	1	Total O S	0	0
			5 4 1		
5	L	1	Total O S	0	0
			5 4 1		
5	L	1	Total O S	0	0
			5 4 1		
5	L	1	Total O S	0	0

• Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	Total C O 9 6 3	0	0
6	А	1	Total C O 12 8 4	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	Total C O 10 7 3	0	0
6	В	1	$\begin{array}{c cccc} 10 & 7 & 0 \\ \hline Total & C & O \\ 10 & 7 & 3 \end{array}$	0	0
6	С	1	$\begin{array}{c cccc} 10 & 1 & 0 \\ \hline Total & C & O \\ 13 & 9 & 4 \end{array}$	0	0
6	С	1	Total C O 9 6 3	0	0
6	D	1	Total C O 10 7 3	0	0
6	D	1	Total C O 11 8 3	0	0
6	D	1	Total C O 10 7 3	0	0
6	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 5 & 2 \end{array}$	0	0
6	Е	1	Total C O 12 8 4	0	0
6	Е	1	Total C O 12 8 4	0	0
6	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 8 & 5 & 3 \end{array}$	0	0
6	F	1	Total C O 10 6 4	0	0
6	F	1	Total C O 10 6 4	0	0
6	F	1	Total C O 10 6 4	0	0
6	G	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 9 6 3 \end{array}$	0	0
6	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 4 & 2 \end{array}$	0	0
6	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 4 & 2 \end{array}$	0	0
6	G	1	Total C O 12 8 4	0	0
6	Н	1	$\begin{array}{c c} \text{Total} & \text{C} & \text{O} \\ 10 & 7 & 3 \end{array}$	0	0
6	Н	1	$\begin{array}{c cc} \hline \text{Total} & \text{C} & \text{O} \\ \hline 10 & 7 & 3 \end{array}$	0	0
6	Ι	1	Total C O 15 10 5	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Ι	1	Total C O 11 8 3	0	0
6	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 5 & 2 \end{array}$	0	0
6	J	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 4 & 2 \end{array}$	0	0
6	J	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 9 6 3 \end{array}$	0	0
6	J	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 9 6 3 \end{array}$	0	0
6	K	1	Total C O 12 8 4	0	0
6	K	1	Total C O 12 8 4	0	0
6	K	1	Total C O 11 7 4	0	0
6	K	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 4 & 2 \end{array}$	0	0
6	L	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
6	L	1	Total C O 10 6 4	0	0
6	L	1	Total C O 12 8 4	0	0
6	L	1	Total C O 11 7 4	0	0
6	L	1	Total C O 12 8 4	0	0

• Molecule 7 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).





Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
7	Δ	1	Total	С	0	S	0	0
	Л	T	4	2	1	1	0	0
7	Δ	1	Total	С	Ο	\mathbf{S}	0	0
-	11	I	4	2	1	1	0	0
7	В	1	Total	С	Ο	\mathbf{S}	0	0
-	D	I	4	2	1	1	0	0
7	С	1	Total	С	Ο	\mathbf{S}	0	0
-	0	I	4	2	1	1	0	0
7	Л	1	Total	С	Ο	\mathbf{S}	0	0
	D	T	4	2	1	1	0	0
7	E	1	Total	С	Ο	\mathbf{S}	0	0
-		1	4	2	1	1	0	0
7	G	1	Total	С	Ο	\mathbf{S}	0	0
		1	4	2	1	1	0	0
7	I	1	Total	С	Ο	\mathbf{S}	0	0
		, I	4	2	1	1		0
7	K	1	Total	С	Ο	\mathbf{S}	0	0
'	11		4	2	1	1		

• Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
8	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	330	Total O 330 330	0	0
9	В	326	Total O 326 326	0	0
9	С	356	Total O 356 356	0	0
9	D	318	Total O 318 318	0	0
9	Е	363	Total O 363 363	0	0
9	F	318	Total O 318 318	0	0
9	G	351	Total O 351 351	0	0
9	Н	283	Total O 283 283	0	0
9	Ι	350	Total O 350 350	0	0
9	J	331	Total O 331 331	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	K	367	Total O 367 367	0	0
9	L	307	Total O 307 307	0	0



Residue-property plots (i) 3

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: Pf-M17

• Molecule 1: Pf-M17





• Molecule 1: Pf-M17





HIS

• Molecule 1: Pf-M17

Chain L: 90%								8%	ó	,																						
ALA S86	0113	V132	P135 GI V	K137 F138	V142	E155	L169	D180	81 04		E200 A201	D202	POOR	V206		T241	THR	ASP	ASN	VAL	MET	E262	Y288	K320 L321	0001	1327	L328	F354	V372	N384	A387 A388	
D394 L395	F398	Y411	K436	Y439 P440	P441	K451	N457	L466	D483	S498	P523		Y533	T536	D543	1544	E564	пеле	HIS	HIS	SIH											



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	174.18Å 177.87Å 229.65Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	44.77 - 2.10	Depositor
Resolution (A)	44.77 - 2.10	EDS
% Data completeness	99.1 (44.77-2.10)	Depositor
(in resolution range)	99.4 (44.77-2.10)	EDS
R _{merge}	0.51	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.97 (at 2.10 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
D D.	0.193 , 0.240	Depositor
n, n_{free}	0.200 , 0.245	DCC
R_{free} test set	20510 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	16.0	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34, 54.8	EDS
L-test for twinning ²	$< L >=0.48, < L^2>=0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	52312	wwPDB-VP
Average B, all atoms $(Å^2)$	20.0	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 46.70 % 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 1.1034e-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: J1V, SO4, ZN, 1PE, DMS, CO3, EDO

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			
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	А	0.40	0/4075	0.54	0/5526		
1	В	0.39	0/4030	0.55	0/5471		
1	С	0.40	0/4076	0.54	0/5530		
1	D	0.40	0/4039	0.54	0/5476		
1	Ε	0.40	0/3989	0.55	0/5411		
1	F	0.38	0/3970	0.54	0/5393		
1	G	0.40	0/4074	0.54	0/5524		
1	Н	0.40	0/4042	0.55	0/5488		
1	Ι	0.40	0/4070	0.55	0/5524		
1	J	0.40	0/4004	0.55	0/5427		
1	Κ	0.42	0/3976	0.56	0/5393		
1	L	0.40	0/3986	0.54	0/5412		
All	All	0.40	0/48331	0.55	0/65575		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3994	0	3928	27	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	3952	0	3869	29	0
1	С	3994	0	3930	20	0
1	D	3955	0	3903	26	0
1	Е	3912	0	3848	40	0
1	F	3890	0	3792	26	0
1	G	3993	0	3936	30	0
1	Н	3960	0	3873	21	0
1	Ι	3992	0	3903	21	0
1	J	3927	0	3888	29	0
1	K	3900	0	3833	33	0
1	L	3910	0	3818	30	0
2	А	4	0	0	0	0
2	В	4	0	0	0	0
2	С	4	0	0	0	0
2	D	4	0	0	0	0
2	Е	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	Н	4	0	0	0	0
2	Ι	4	0	0	0	0
2	J	4	0	0	0	0
2	K	4	0	0	0	0
2	L	4	0	0	0	0
3	A	1	0	0	0	0
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	l	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	29	0	0	0	0
4	B	29	0	0	1	0
4		29	0	0	0	0
4	D	29	0	0	2	0
4		29	0	0	1	0
4	F'	29	0	0	0	0
4	G	29	0	0	1	0



	Chain	Non-H	H(model)	H(addad)	Clashes	Symm-Clashes
	Ц	20				
4	II	29	0	0	0	0
4	I	29	0	0	0	0
4	J K	29	0	0	1	0
4	L	29	0	0	0	0
5		$\frac{23}{25}$	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	10	0	0	1	0
5	E E	10	0	0	1	0
5	F	5	0	0	0	0
5	G	15	0	0	1	0
5	I	10	0	0	0	0
5	K I	15	0	0	0	0
5	L	15	0	0	0	0
6	A	21	0	22	2	0
6	B	20	0	22	2	0
6	C	20	0	20	1	0
6	D	38	0	38	3	0
6	E	32	0	36	1	0
6	F	30	0	39	6	0
6	G	33	0	34	3	0
6	H	20	0	20	2	0
6	Ι	33	0	37	6	0
6	J	24	0	20	1	0
6	K	41	0	44	4	0
6	L	52	0	63	12	0
7	А	8	0	12	5	0
7	В	4	0	6	0	0
7	С	4	0	6	0	0
7	D	4	0	6	1	0
7	Е	4	0	6	1	0
7	G	4	0	6	2	0
7	J	4	0	6	0	0
7	K	4	0	6	0	0
8	Ι	8	0	12	0	0
9	А	330	0	0	0	0
9	В	326	0	0	3	0
9	С	356	0	0	6	0
9	D	318	0	0	2	0
9	Е	363	0	0	9	0
9	F	318	0	0	3	0

 α J fa ntina



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	G	351	0	0	4	0
9	Н	283	0	0	2	0
9	Ι	350	0	0	3	0
9	J	331	0	0	4	0
9	Κ	367	0	0	5	0
9	L	307	0	0	1	0
All	All	52312	0	46984	311	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 311 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)
4:D:703:J1V:NAR	4:D:703:J1V:OAC	1.58	1.31
1:B:116:ASP:OD2	1:B:118:LYS:HE2	1.69	0.91
1:L:457:ASN:HD21	6:L:709:1PE:H162	1.36	0.90
9:I:855:HOH:O	1:K:164:LYS:HE3	1.72	0.88
1:B:131:LEU:HD21	1:B:224:VAL:HG13	1.60	0.83

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	518/526~(98%)	504 (97%)	14 (3%)	0	100	100
1	В	517/526~(98%)	505~(98%)	12 (2%)	0	100	100
1	С	519/526~(99%)	510 (98%)	9~(2%)	0	100	100
1	D	514/526~(98%)	504 (98%)	10 (2%)	0	100	100
1	Ε	506/526~(96%)	495 (98%)	11 (2%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	F	505/526~(96%)	495~(98%)	10 (2%)	0	100	100
1	G	518/526~(98%)	507~(98%)	11 (2%)	0	100	100
1	Н	519/526~(99%)	504 (97%)	13~(2%)	2~(0%)	34	32
1	Ι	521/526~(99%)	511 (98%)	8 (2%)	2~(0%)	34	32
1	J	508/526~(97%)	497~(98%)	11 (2%)	0	100	100
1	K	503/526~(96%)	495~(98%)	8 (2%)	0	100	100
1	L	507/526~(96%)	492 (97%)	15(3%)	0	100	100
All	All	6155/6312 (98%)	6019 (98%)	132 (2%)	4 (0%)	51	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Н	258	ASN
1	Ι	606	HIS
1	Ι	607	HIS
1	Н	259	VAL

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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles			
1	А	429/453~(95%)	424 (99%)	5 (1%)	71	77		
1	В	417/453~(92%)	409 (98%)	8 (2%)	57	63		
1	С	428/453~(94%)	421 (98%)	7~(2%)	62	69		
1	D	420/453~(93%)	414 (99%)	6 (1%)	67	73		
1	Ε	418/453~(92%)	415 (99%)	3~(1%)	84	88		
1	F	413/453 (91%)	406 (98%)	7(2%)	60	67		
1	G	429/453~(95%)	424 (99%)	5(1%)	71	77		
1	Н	418/453~(92%)	412 (99%)	6 (1%)	67	73		
1	Ι	425/453~(94%)	420 (99%)	5 (1%)	71	77		



Mol	Chain	Analysed	Rotameric	Rotameric Outliers		Percentiles		
1	J	420/453~(93%)	418 (100%)	2~(0%)	88	92		
1	Κ	416/453~(92%)	410 (99%)	6 (1%)	67	73		
1	L	416/453~(92%)	411 (99%)	5 (1%)	71	77		
All	All	5049/5436~(93%)	4984 (99%)	65 (1%)	71	75		

Continued from previous page...

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Κ	439	TYR
1	Κ	550	SER
1	D	439[A]	TYR
1	D	400[B]	MET
1	L	113	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 107 ligands modelled in this entry, $12~{\rm are}$ monoatomic - leaving 95 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



Mol	Turno	Chain	Dog	Link	Bo	ond leng	ths	В	ond ang	les
MOI	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	D	705	-	4,4,4	0.17	0	$6,\!6,\!6$	0.17	0
5	SO4	G	704	-	4,4,4	0.15	0	$6,\!6,\!6$	0.33	0
6	1PE	F	707	-	9,9,15	0.70	0	8,8,14	0.27	0
7	DMS	А	709	-	3,3,3	0.79	0	3,3,3	0.78	0
6	1PE	L	707	-	11,11,15	0.74	0	10,10,14	0.32	0
6	1PE	G	707	-	$5,\!5,\!15$	0.61	0	4,4,14	0.48	0
5	SO4	Ι	710	-	4,4,4	0.30	0	$6,\!6,\!6$	0.36	0
7	DMS	K	709	-	3,3,3	0.58	0	3, 3, 3	0.67	0
5	SO4	В	707	-	4,4,4	0.15	0	$6,\!6,\!6$	0.09	0
6	1PE	L	708	-	10,10,15	0.69	0	9,9,14	0.24	0
2	CO3	А	701	-	2,3,3	0.39	0	$2,\!3,\!3$	0.93	0
7	DMS	В	706	-	3,3,3	0.64	0	3, 3, 3	0.77	0
6	1PE	D	707	-	10,10,15	0.82	0	$9,\!9,\!14$	0.52	0
7	DMS	А	710	-	3,3,3	0.65	0	3, 3, 3	0.79	0
7	DMS	D	710	-	3,3,3	0.73	0	3, 3, 3	0.64	0
8	EDO	Ι	707	-	3,3,3	0.52	0	$2,\!2,\!2$	0.45	0
4	J1V	L	704	3	31,31,31	1.90	5 (16%)	42,43,43	1.66	9 (21%)
5	SO4	K	711	-	4,4,4	0.12	0	$6,\!6,\!6$	0.32	0
6	1PE	G	706	-	8,8,15	0.68	0	7,7,14	0.24	0
4	J1V	K	703	3	31,31,31	2.02	4 (12%)	42,43,43	1.64	9 (21%)
7	DMS	Е	707	-	3,3,3	0.58	0	3,3,3	0.97	0
6	1PE	Е	706	-	7,7,15	0.69	0	6,6,14	0.43	0
6	1PE	K	706	-	11,11,15	0.71	0	10,10,14	0.42	0
4	J1V	F	703	3	31,31,31	1.94	4 (12%)	42,43,43	1.52	8 (19%)
5	SO4	L	710	-	4,4,4	0.12	0	$6,\!6,\!6$	0.21	0
7	DMS	С	706	-	3,3,3	0.76	0	3,3,3	0.55	0
5	SO4	А	711	-	4,4,4	0.14	0	$6,\!6,\!6$	0.10	0
6	1PE	G	708	-	5,5,15	0.70	0	4,4,14	0.35	0
6	1PE	J	704	-	5,5,15	0.69	0	4,4,14	0.32	0
5	SO4	А	705	-	4,4,4	0.18	0	$6,\!6,\!6$	0.12	0
6	1PE	С	704	-	12,12,15	0.73	0	11,11,14	0.33	0
7	DMS	J	707	-	3,3,3	0.59	0	3, 3, 3	0.68	0
2	CO3	K	701	-	2,3,3	0.29	0	$2,\!3,\!3$	0.47	0
6	1PE	G	709	-	11,11,15	0.73	0	$10,\!10,\!14$	0.28	0
2	CO3	В	701	-	2,3,3	0.55	0	$2,\!3,\!3$	0.96	0
2	CO3	L	702	-	2,3,3	0.38	0	$2,\!3,\!3$	1.13	0
6	1PE	Ι	704	-	14,14,15	0.46	0	13,13,14	0.49	0
6	1PE	D	709	-	6,6,15	0.78	0	$5,\!5,\!14$	0.32	0
6	1PE	Ι	705	-	10,10,15	0.69	0	9,9,14	0.34	0
5	SO4	C	707	-	4,4,4	0.09	0	$6, 6, \overline{6}$	$0.3\overline{5}$	0

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).



	T a	Chain	Dag	T : 1-	Bo	ond leng	ths	В	ond ang	les
IVIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	CO3	F	701	-	2,3,3	0.32	0	2,3,3	0.54	0
2	CO3	Е	701	-	2,3,3	0.40	0	2,3,3	0.41	0
6	1PE	А	706	-	8,8,15	0.68	0	7,7,14	0.25	0
5	SO4	K	704	-	4,4,4	0.13	0	$6,\!6,\!6$	0.14	0
2	CO3	С	701	-	2,3,3	0.53	0	2,3,3	1.34	0
4	J1V	G	703	3	31,31,31	2.10	5 (16%)	42,43,43	1.75	9 (21%)
5	SO4	G	711	-	4,4,4	0.12	0	$6,\!6,\!6$	0.08	0
6	1PE	L	706	-	$9,\!9,\!15$	0.58	0	8,8,14	0.17	0
5	SO4	Е	708	-	4,4,4	0.21	0	$6,\!6,\!6$	0.14	0
6	1PE	K	705	-	11,11,15	0.73	0	10,10,14	0.43	0
4	J1V	D	703	3	31,31,31	2.08	5 (16%)	42,43,43	1.44	7 (16%)
8	EDO	Ι	708	-	3,3,3	0.46	0	2,2,2	0.48	0
6	1PE	Ι	706	-	$6,\!6,\!15$	0.73	0	$5,\!5,\!14$	0.25	0
7	DMS	G	710	-	3,3,3	0.67	0	3,3,3	0.66	0
6	1PE	D	706	-	9,9,15	0.69	0	8,8,14	0.24	0
4	J1V	Н	703	3	31,31,31	1.82	3 (9%)	42,43,43	1.67	8 (19%)
6	1PE	J	706	-	8,8,15	0.74	0	7,7,14	0.44	0
2	CO3	J	701	-	2,3,3	0.53	0	2,3,3	0.73	0
5	SO4	А	704	-	4,4,4	0.12	0	$6,\!6,\!6$	0.12	0
5	SO4	E	709	-	4,4,4	0.20	0	6,6,6	0.15	0
4	J1V	С	703	3	31,31,31	1.75	6 (19%)	42,43,43	1.31	5 (11%)
6	1PE	F	705	-	$9,\!9,\!15$	0.64	0	8,8,14	0.36	0
6	1PE	K	707	-	10,10,15	0.78	0	$9,\!9,\!14$	0.32	0
2	CO3	Ι	702	-	2,3,3	0.36	0	2,3,3	1.08	0
6	1PE	K	708	-	5,5,15	0.77	0	4,4,14	0.35	0
6	1PE	L	701	-	6,6,15	0.72	0	$5,\!5,\!14$	0.32	0
6	1PE	E	705	-	11,11,15	0.69	0	10,10,14	0.27	0
5	SO4	A	708	-	4,4,4	0.20	0	6,6,6	0.17	0
5	SO4	A	712	-	4,4,4	0.13	0	6,6,6	0.09	0
2	CO3	H	701	-	2,3,3	0.46	0	2,3,3	0.78	0
4	J1V	A	703	3	31,31,31	2.05	4 (12%)	42,43,43	1.76	9 (21%)
5	SO4	K	710		4,4,4	0.18	0	6,6,6	0.23	0
4	J1V	E	703	3	31,31,31	2.02	5(16%)	42,43,43	1.39	7(16%)
6	1PE	В	705	-	9,9,15	0.75	0	8,8,14	0.53	0
4	J1V	J	703	3	31,31,31	1.96	5 (16%)	42,43,43	1.37	6 (14%)
5	SO4	Ι	709	-	4,4,4	0.14	0	6,6,6	0.26	0
6	1PE	Н	704	-	9,9,15	0.68	0	8,8,14	0.39	0
5	SO4	L	711	-	4,4,4	0.13	0	6,6,6	0.13	0
6	1PE	E	704	-	11,11,15	0.72	0	10,10,14	0.34	0
5	SO4	G	705		4,4,4	0.13	0	6,6,6	0.17	0
6	1PE	C	705		8,8,15	0.68	0	7,7,14	0.33	0



Mal	Iol Type Chain Res Link		Tink	Bo	ond leng	$_{\rm ths}$	Bond angles			
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
6	1PE	F	706	-	9,9,15	0.67	0	8,8,14	0.23	0
4	J1V	Ι	703	3	31,31,31	1.73	3 (9%)	42,43,43	1.47	7 (16%)
5	SO4	F	704	-	4,4,4	0.11	0	$6,\!6,\!6$	0.18	0
2	CO3	D	701	-	2,3,3	0.44	0	2,3,3	0.56	0
6	1PE	А	707	-	11,11,15	0.74	0	10,10,14	0.28	0
2	CO3	G	701	-	2,3,3	0.45	0	2,3,3	0.66	0
6	1PE	Н	705	-	9,9,15	0.78	0	8,8,14	0.39	0
6	1PE	D	708	-	9,9,15	0.77	0	8,8,14	0.41	0
6	1PE	J	705	-	8,8,15	0.68	0	7,7,14	0.30	0
6	1PE	L	709	-	11,11,15	0.78	0	10,10,14	0.66	0
6	1PE	В	704	-	9,9,15	0.72	0	8,8,14	0.28	0
5	SO4	D	704	-	4,4,4	0.17	0	$6,\!6,\!6$	0.05	0
4	J1V	В	703	3	31,31,31	1.73	3 (9%)	42,43,43	1.46	7 (16%)
5	SO4	L	705	-	4,4,4	0.16	0	$6,\!6,\!6$	0.18	0

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
6	1PE	С	704	-	-	5/10/10/13	-
6	1PE	К	705	-	-	2/9/9/13	-
4	J1V	D	703	3	-	4/22/30/30	0/3/3/3
4	J1V	J	703	3	-	4/22/30/30	0/3/3/3
8	EDO	Ι	708	-	-	0/1/1/1	-
6	1PE	Ι	706	-	-	3/4/4/13	-
6	1PE	F	707	-	-	2/7/7/13	-
6	1PE	D	706	-	-	6/7/7/13	-
4	J1V	Н	703	3	-	3/22/30/30	0/3/3/3
6	1PE	J	706	-	-	5/6/6/13	-
6	1PE	L	707	-	-	7/9/9/13	-
6	1PE	G	707	-	-	2/3/3/13	-
6	1PE	Н	704	-	-	0/7/7/13	-
6	1PE	G	709	-	-	5/9/9/13	-
6	1PE	Е	704	-	-	3/9/9/13	-
4	J1V	С	703	3	-	3/22/30/30	0/3/3/3
6	1PE	F	705	-	-	2/7/7/13	-
6	1PE	Ι	704	-	-	6/12/12/13	-



Conti	nuea fro	m previoi	is page				
Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	L	708	-	-	4/8/8/13	-
6	1PE	С	705	-	-	5/6/6/13	-
8	EDO	Ι	707	-	-	1/1/1/1	-
6	1PE	D	707	-	-	3/8/8/13	-
6	1PE	D	709	-	-	4/4/4/13	-
6	1PE	Ι	705	-	-	5/8/8/13	-
6	1PE	K	707	-	-	4/8/8/13	-
6	1PE	F	706	-	-	3/7/7/13	-
4	J1V	L	704	3	-	5/22/30/30	0/3/3/3
6	1PE	К	708	-	-	3/3/3/13	-
4	J1V	Ι	703	3	-	4/22/30/30	0/3/3/3
6	1PE	L	701	-	-	3/4/4/13	-
6	1PE	Е	705	-	-	3/9/9/13	-
6	1PE	А	707	-	-	4/9/9/13	-
6	1PE	G	706	-	-	5/6/6/13	-
4	J1V	K	703	3	-	3/22/30/30	0/3/3/3
6	1PE	Н	705	-	-	1/7/7/13	-
6	1PE	D	708	-	-	2/7/7/13	-
6	1PE	J	705	-	-	4/6/6/13	-
6	1PE	Е	706	-	-	3/5/5/13	-
6	1PE	L	709	-	-	5/9/9/13	-
6	1PE	K	706	-	-	4/9/9/13	-
6	1PE	А	706	-	-	2/6/6/13	-
4	J1V	F	703	3	-	4/22/30/30	0/3/3/3
6	1PE	В	704	-	-	1/7/7/13	-
6	1PE	G	708	-	-	2/3/3/13	-
6	1PE	J	704	-	-	1/3/3/13	-
4	J1V	А	703	3	-	3/22/30/30	0/3/3/3
4	J1V	В	703	3	-	4/22/30/30	0/3/3/3
4	J1V	G	703	3	-	3/22/30/30	0/3/3/3
6	1PE	L	706	-	-	4/7/7/13	-
4	J1V	E	703	3	-	4/22/30/30	0/3/3/3
6	1PE	В	705	-	-	4/7/7/13	-

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The worst 5 of 52 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
4	Κ	703	J1V	CAZ-CA	-8.67	1.38	1.52
4	Н	703	J1V	CAZ-CA	-8.40	1.39	1.52
4	G	703	J1V	CAZ-CA	-8.26	1.39	1.52
4	Е	703	J1V	CAZ-CA	-8.11	1.39	1.52
4	F	703	J1V	CAZ-CA	-8.11	1.39	1.52

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	Н	703	J1V	CAJ-CAZ-CA	-3.95	114.31	120.80
4	Н	703	J1V	CAG-CAI-CAZ	-3.92	117.25	121.20
4	L	704	J1V	CAJ-CAZ-CA	-3.92	114.36	120.80
4	А	703	J1V	O-C-NAR	3.82	128.21	123.27
4	Κ	703	J1V	CAN-CAP-CBB	-3.63	104.45	111.33

There are no chirality outliers.

5 of 172 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	703	J1V	N-CAU-CBB-CAP
6	L	709	1PE	C25-C15-OH6-C26
6	L	706	1PE	OH6-C15-C25-OH5
6	L	709	1PE	OH6-C15-C25-OH5
6	С	705	1PE	OH4-C13-C23-OH3

There are no ring outliers.

34 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	705	SO4	1	0
6	F	707	1PE	1	0
7	А	709	DMS	3	0
6	L	707	1PE	4	0
6	G	707	1PE	1	0
6	D	707	1PE	1	0
7	А	710	DMS	2	0
7	D	710	DMS	1	0
4	K	703	J1V	1	0
7	Е	707	DMS	1	0
6	Е	706	1PE	1	0
6	K	706	1PE	1	0
6	G	709	1PE	2	0



Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Ι	704	1PE	5	0
6	Ι	705	1PE	1	0
4	G	703	J1V	1	0
6	L	706	1PE	1	0
4	D	703	J1V	2	0
7	G	710	DMS	2	0
6	D	706	1PE	1	0
5	Ε	709	SO4	1	0
6	Κ	707	1PE	2	0
6	Κ	708	1PE	1	0
4	Ε	703	J1V	1	0
6	В	705	1PE	2	0
5	G	705	SO4	1	0
6	С	705	1PE	1	0
6	F	706	1PE	5	0
6	А	707	1PE	2	0
6	Н	705	1PE	2	0
6	D	708	1PE	1	0
6	J	705	1PE	1	0
6	L	709	1PE	7	0
4	В	703	J1V	1	0

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 sufficient must be 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	OWAB(Å ²)	Q<0.9
1	А	519/526~(98%)	-0.51	5 (0%) 82 85	9, 17, 34, 57	3~(0%)
1	В	518/526~(98%)	-0.42	7 (1%) 75 78	9, 19, 44, 62	4 (0%)
1	С	520/526~(98%)	-0.53	3 (0%) 89 91	9, 17, 35, 51	7 (1%)
1	D	516/526~(98%)	-0.44	7 (1%) 75 78	10, 17, 34, 84	12 (2%)
1	Ε	510/526~(96%)	-0.65	0 100 100	9, 16, 29, 44	9 (1%)
1	F	510/526~(96%)	-0.42	0 100 100	11, 20, 38, 49	8 (1%)
1	G	519/526~(98%)	-0.54	2 (0%) 92 93	9, 17, 33, 52	6 (1%)
1	Н	520/526~(98%)	-0.44	8 (1%) 73 77	9, 18, 45, 74	10 (1%)
1	Ι	523/526~(99%)	-0.52	4 (0%) 86 88	9, 17, 35, 61	6 (1%)
1	J	512/526~(97%)	-0.48	2 (0%) 92 93	9, 17, 34, 53	8 (1%)
1	Κ	509/526~(96%)	-0.64	1 (0%) 95 95	10, 16, 29, 50	5~(0%)
1	L	513/526~(97%)	-0.47	1 (0%) 95 95	9, 18, 37, 48	13 (2%)
All	All	6189/6312 (98%)	-0.51	40 (0%) 89 91	9, 17, 37, 84	91 (1%)

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	259	VAL	5.1
1	J	85	ALA	4.1
1	D	260	ASN	3.8
1	В	136	GLY	3.7
1	D	603	ASP	3.4

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	$B-factors(A^2)$	Q<0.9
6	1PE	K	707	11/16	0.71	0.27	33,37,45,50	0
7	DMS	А	710	4/4	0.76	0.17	18,28,52,59	0
5	SO4	А	705	5/5	0.78	0.18	60,63,78,83	0
6	1PE	L	709	12/16	0.79	0.32	25,32,38,51	0
6	1PE	F	706	10/16	0.79	0.18	41,46,49,52	0
6	1PE	Е	706	8/16	0.80	0.25	31,38,39,43	0
6	1PE	K	708	6/16	0.80	0.14	25,32,40,43	0
6	1PE	L	701	7/16	0.80	0.18	24,35,43,45	0
6	1PE	G	709	12/16	0.80	0.17	30,47,52,57	0
6	1PE	Н	705	10/16	0.80	0.18	30,43,46,47	0
5	SO4	Е	709	5/5	0.81	0.33	53,53,55,58	5
6	1PE	А	707	12/16	0.81	0.19	33,43,49,53	0
6	1PE	D	707	11/16	0.81	0.42	31,39,45,46	0
6	1PE	D	709	7/16	0.82	0.17	18,25,33,34	0
6	1PE	С	704	13/16	0.82	0.24	27,41,49,54	0
6	1PE	Ι	704	15/16	0.82	0.22	27,40,49,55	0
6	1PE	D	708	10/16	0.82	0.17	27,36,45,49	0
7	DMS	Е	707	4/4	0.82	0.19	23,28,43,46	0
7	DMS	K	709	4/4	0.82	0.21	27,36,38,52	0
6	1PE	L	708	11/16	0.83	0.19	38,45,50,52	0
6	1PE	K	705	12/16	0.84	0.14	35,38,46,47	0
6	1PE	В	705	10/16	0.84	0.14	30,34,42,43	0
5	SO4	Ι	710	5/5	0.84	0.40	52,59,67,68	5
6	1PE	J	706	9/16	0.85	0.16	29,37,41,43	0
6	1PE	J	704	6/16	0.85	0.19	21,27,34,36	0
6	1PE	Е	704	12/16	0.86	0.17	30,34,41,42	0
7	DMS	G	710	4/4	0.86	0.18	19,19,27,40	0
6	1PE	F	707	10/16	0.86	0.22	28,39,44,44	0
5	SO4	Е	708	5/5	0.87	0.27	28,41,46,48	5
6	1PE	L	707	12/16	0.87	0.28	30,41,51,53	0
8	EDO	Ι	707	4/4	0.87	0.12	24,26,30,35	0
6	1PE	Ι	705	11/16	0.88	0.12	$2\overline{5,}27,\!41,\!44$	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
7	DMS	С	706	4/4	0.88	0.21	28,29,35,44	0
6	1PE	G	708	6/16	0.88	0.14	23,31,34,34	0
6	1PE	G	706	9/16	0.89	0.14	26,29,41,41	0
5	SO4	А	712	5/5	0.90	0.32	81,84,87,87	0
6	1PE	F	705	10/16	0.90	0.11	25,30,35,35	0
6	1PE	Ι	706	7/16	0.90	0.14	24,33,36,37	0
6	1PE	С	705	9/16	0.90	0.13	17,22,34,37	0
6	1PE	Н	704	10/16	0.90	0.12	25,29,38,40	0
5	SO4	L	710	5/5	0.90	0.23	45,46,49,51	5
5	SO4	D	704	5/5	0.91	0.29	62,62,65,80	0
5	SO4	А	711	5/5	0.91	0.28	63,64,72,76	0
4	J1V	K	703	29/29	0.91	0.11	16,24,31,33	0
7	DMS	D	710	4/4	0.91	0.16	21,31,36,39	0
4	J1V	D	703	29/29	0.92	0.11	17,24,36,39	0
6	1PE	G	707	6/16	0.92	0.14	31,32,34,38	0
6	1PE	J	705	9/16	0.92	0.10	19,26,30,30	0
4	J1V	Е	703	29/29	0.92	0.10	18,23,32,33	0
4	J1V	F	703	29/29	0.92	0.12	17,22,32,36	0
4	J1V	J	703	29/29	0.92	0.12	17,22,31,31	0
3	ZN	J	702	1/1	0.92	0.07	45,45,45,45	1
6	1PE	D	706	10/16	0.92	0.11	23,29,35,36	0
4	J1V	С	703	29/29	0.92	0.11	14,24,34,38	0
7	DMS	А	709	4/4	0.93	0.18	26,28,41,49	0
4	J1V	Н	703	29/29	0.93	0.12	14,20,34,40	0
7	DMS	В	706	4/4	0.93	0.20	$26,\!26,\!34,\!45$	0
4	J1V	А	703	29/29	0.93	0.12	17,22,32,33	0
6	1PE	А	706	9/16	0.93	0.12	19,28,32,33	0
6	1PE	L	706	10/16	0.93	0.13	21,32,38,46	0
4	J1V	В	703	29/29	0.93	0.12	$17,\!22,\!31,\!34$	0
6	1PE	В	704	10/16	0.93	0.12	$21,\!28,\!42,\!51$	0
5	SO4	Ι	709	5/5	0.93	0.15	42,49,50,53	5
4	J1V	Ι	703	29/29	0.94	0.10	16,23,30,31	0
5	SO4	L	705	5/5	0.94	0.31	$50,\!58,\!63,\!81$	0
4	J1V	L	704	29/29	0.94	0.11	$15,\!24,\!31,\!32$	0
6	1PE	E	705	12/16	0.94	0.15	$23,\!28,\!42,\!45$	0
5	SO4	L	711	5/5	0.94	0.25	44,54,57,62	0
5	SO4	F	704	5/5	0.94	0.22	52,53,58,70	0
4	J1V	G	703	29/29	0.94	0.11	16,23,32,41	0
6	1PE	K	706	$12/\overline{16}$	0.94	0.14	23,27,45,48	0
8	EDO	Ι	708	4/4	0.94	0.11	31,33,34,35	0
5	SO4	A	704	5/5	0.95	0.23	46,54,66,66	0
5	SO4	B	707	5/5	0.95	0.35	40,50,53,53	5



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	С	707	5/5	0.95	0.20	22,26,27,32	5
2	CO3	D	701	4/4	0.95	0.09	$13,\!15,\!19,\!22$	0
5	SO4	Κ	704	5/5	0.95	0.28	63,68,71,77	0
5	SO4	Κ	710	5/5	0.95	0.16	25,29,37,38	5
2	CO3	В	701	4/4	0.95	0.11	13,13,15,20	0
2	CO3	L	702	4/4	0.96	0.11	13,14,16,21	0
3	ZN	F	702	1/1	0.96	0.04	40,40,40,40	1
2	CO3	С	701	4/4	0.96	0.10	13,15,20,23	0
7	DMS	J	707	4/4	0.96	0.14	25,25,33,36	0
2	CO3	G	701	4/4	0.96	0.09	12,15,18,29	0
2	CO3	Ι	702	4/4	0.96	0.10	13,14,16,22	0
5	SO4	G	711	5/5	0.96	0.28	57,59,63,66	0
3	ZN	В	702	1/1	0.97	0.06	42,42,42,42	1
3	ZN	Е	702	1/1	0.97	0.07	45,45,45,45	1
2	CO3	J	701	4/4	0.97	0.09	11,11,16,23	0
3	ZN	Н	702	1/1	0.97	0.05	41,41,41,41	1
3	ZN	Ι	701	1/1	0.97	0.06	44,44,44,44	1
2	CO3	А	701	4/4	0.97	0.12	8,13,14,25	0
5	SO4	G	705	5/5	0.97	0.15	49,49,56,57	0
3	ZN	Κ	702	1/1	0.97	0.05	44,44,44,44	1
3	ZN	L	703	1/1	0.97	0.03	41,41,41,41	1
2	CO3	Н	701	4/4	0.98	0.08	$10,\!15,\!20,\!22$	0
2	CO3	F	701	4/4	0.98	0.05	14,15,21,22	0
3	ZN	D	702	1/1	0.98	0.04	41,41,41,41	1
2	CO3	Е	701	4/4	0.98	0.09	$13,\!13,\!18,\!19$	0
2	CO3	Κ	701	4/4	0.98	0.08	12,15,17,20	0
3	ZN	G	702	1/1	0.98	0.04	39,39,39,39	1
5	SO4	Κ	711	5/5	0.99	0.08	15,16,20,21	0
3	ZN	А	702	1/1	0.99	0.05	40,40,40,40	1
3	ZN	С	702	1/1	0.99	0.04	37,37,37,37	1
5	SO4	D	705	5/5	0.99	0.09	12, 14, 15, 17	0
5	SO4	А	708	5/5	1.00	0.06	$13,\!13,\!17,\!18$	0
5	SO4	G	704	5/5	1.00	0.05	$10,\!10,\!13,\!15$	0

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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.

