

Full wwPDB X-ray Structure Validation Report (i)

Dec 25, 2023 – 04:40 PM JST

PDB ID	:	8WWV
Title	:	1-naphthylamine GS in complex with ADP and MetSox-P
Authors	:	Zhang, S.T.; Zhou, N.Y.
Deposited on	:	2023-10-26
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* 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 2.30 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	5042(2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575(2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	Δ	F10	9%		_
L	A	510	87%	8%	•
			9%		_
1	В	510	86%	10%	·
			5%		
1	C	510	87%	9%	•
			3%		
1	D	510	88%	8%	•
			4%		
1	Ε	510	89%	7%	•
			6%		
1	F	510	85%	10%	•



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 46408 atoms, of which 22530 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	Δ	400	Total	С	Η	Ν	0	\mathbf{S}	0	0	0
	A	490	7565	2439	3737	643	728	18	0	0	0
1	P	199	Total	С	Η	Ν	0	S	0	0	0
	D	400	7524	2434	3705	641	726	18	0	0	0
1	С	400	Total	С	Η	Ν	0	S	0	0	0
	U	490	7560	2439	3732	643	728	18	0	0	0
1	Л	400	Total	С	Η	Ν	0	S	0	0	0
	D	490	7552	2439	3724	643	728	18	0	0	0
1	F	480	Total	С	Η	Ν	0	S	0	0	0
		409	7571	2435	3751	642	725	18	0	0	0
1	1 F	400	Total	С	Η	Ν	0	\mathbf{S}	0	0	0
		490	7583	2439	3755	643	728	18		U	0

• Molecule 1 is a protein called Glutamine synthetase.

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-14	TRP	-	expression tag	UNP A0A7Y1Q2L1
А	-13	SER	-	expression tag	UNP A0A7Y1Q2L1
А	-12	HIS	-	expression tag	UNP A0A7Y1Q2L1
А	-11	PRO	-	expression tag	UNP A0A7Y1Q2L1
А	-10	GLN	-	expression tag	UNP A0A7Y1Q2L1
А	-9	PHE	-	expression tag	UNP A0A7Y1Q2L1
А	-8	GLU	-	expression tag	UNP A0A7Y1Q2L1
А	-7	LYS	-	expression tag	UNP A0A7Y1Q2L1
А	-6	GLU	-	expression tag	UNP A0A7Y1Q2L1
А	-5	ASN	-	expression tag	UNP A0A7Y1Q2L1
А	-4	LEU	-	expression tag	UNP A0A7Y1Q2L1
А	-3	TYR	-	expression tag	UNP A0A7Y1Q2L1
А	-2	PHE	-	expression tag	UNP A0A7Y1Q2L1
A	-1	GLN	-	expression tag	UNP A0A7Y1Q2L1
А	0	GLY	-	expression tag	UNP A0A7Y1Q2L1
A	3	ARG	GLN	conflict	UNP A0A7Y1Q2L1
А	69	ALA	THR	conflict	UNP A0A7Y1Q2L1



Chain	Residue	Modelled	Actual	Comment	Reference
А	70	ILE	MET	conflict	UNP A0A7Y1Q2L1
А	71	GLY	ALA	conflict	UNP A0A7Y1Q2L1
А	81	MET	ILE	conflict	UNP A0A7Y1Q2L1
А	85	LEU	PRO	conflict	UNP A0A7Y1Q2L1
А	88	THR	ALA	conflict	UNP A0A7Y1Q2L1
А	89	ALA	GLY	conflict	UNP A0A7Y1Q2L1
А	91	ASP	GLY	conflict	UNP A0A7Y1Q2L1
А	?	-	GLY	deletion	UNP A0A7Y1Q2L1
А	93	GLU	ILE	conflict	UNP A0A7Y1Q2L1
А	99	ASN	SER	conflict	UNP A0A7Y1Q2L1
А	101	THR	SER	conflict	UNP A0A7Y1Q2L1
А	201	VAL	TYR	conflict	UNP A0A7Y1Q2L1
А	314	LEU	VAL	conflict	UNP A0A7Y1Q2L1
А	363	LYS	ARG	conflict	UNP A0A7Y1Q2L1
А	370	VAL	ILE	conflict	UNP A0A7Y1Q2L1
В	-14	TRP	-	expression tag	UNP A0A7Y1Q2L1
В	-13	SER	-	expression tag	UNP A0A7Y1Q2L1
В	-12	HIS	-	expression tag	UNP A0A7Y1Q2L1
В	-11	PRO	-	expression tag	UNP A0A7Y1Q2L1
В	-10	GLN	-	expression tag	UNP A0A7Y1Q2L1
В	-9	PHE	-	expression tag	UNP A0A7Y1Q2L1
В	-8	GLU	-	expression tag	UNP A0A7Y1Q2L1
В	-7	LYS	-	expression tag	UNP A0A7Y1Q2L1
В	-6	GLU	-	expression tag	UNP A0A7Y1Q2L1
В	-5	ASN	-	expression tag	UNP A0A7Y1Q2L1
В	-4	LEU	-	expression tag	UNP A0A7Y1Q2L1
В	-3	TYR	-	expression tag	UNP A0A7Y1Q2L1
В	-2	PHE	-	expression tag	UNP A0A7Y1Q2L1
B	-1	GLN	-	expression tag	UNP A0A7Y1Q2L1
B	0	GLY	-	expression tag	UNP A0A7Y1Q2L1
В	3	ARG	GLN	conflict	UNP A0A7Y1Q2L1
B	69	ALA	THR	conflict	UNP A0A7Y1Q2L1
B	70	ILE	MET	conflict	UNP A0A7Y1Q2L1
B	71	GLY	ALA	conflict	UNP A0A7Y1Q2L1
В	81	MET	ILE	conflict	UNP A0A7Y1Q2L1
B	85	LEU	PRO	conflict	UNP A0A7Y1Q2L1
B	88	THR	ALA	conflict	UNP A0A7Y1Q2L1
B	89	ALA	GLY	conflict	UNP A0A7Y1Q2L1
B	91	ASP	GLY	conflict	UNP A0A7Y1Q2L1
B	?	-	GLY	deletion	UNP A0A7Y1Q2L1
B	93	GLU	ILE	conflict	UNP A0A7Y1Q2L1
B	99	ASN	SER	conflict	UNP A0A7Y1Q2L1



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Chain	Residue	Modelled	Actual	Comment	Reference		
B	101	THR	SER	conflict	UNP A0A7Y1Q2L1		
B	201	VAL	TYR	conflict	UNP A0A7Y1Q2L1		
B	314	LEU	VAL	conflict	UNP A0A7Y1Q2L1		
В	363	LYS	ARG	conflict	UNP A0A7Y1Q2L1		
В	370	VAL	ILE	conflict	UNP A0A7Y1Q2L1		
C	-14	TRP	-	expression tag	UNP A0A7Y1Q2L1		
С	-13	SER	-	expression tag	UNP A0A7Y1Q2L1		
C	-12	HIS	-	expression tag	UNP A0A7Y1Q2L1		
С	-11	PRO	-	expression tag	UNP A0A7Y1Q2L1		
C	-10	GLN	-	expression tag	UNP A0A7Y1Q2L1		
С	-9	PHE	-	expression tag	UNP A0A7Y1Q2L1		
C	-8	GLU	-	expression tag	UNP A0A7Y1Q2L1		
C	-7	LYS	-	expression tag	UNP A0A7Y1Q2L1		
С	-6	GLU	-	expression tag	UNP A0A7Y1Q2L1		
С	-5	ASN	-	expression tag	UNP A0A7Y1Q2L1		
С	-4	LEU	-	expression tag	UNP A0A7Y1Q2L1		
С	-3	TYR	-	expression tag	UNP A0A7Y1Q2L1		
С	-2	PHE	-	expression tag	UNP A0A7Y1Q2L1		
С	-1	GLN	-	expression tag	UNP A0A7Y1Q2L1		
С	0	GLY	-	expression tag	UNP A0A7Y1Q2L1		
С	3	ARG	GLN	conflict	UNP A0A7Y1Q2L1		
С	69	ALA	THR	conflict	UNP A0A7Y1Q2L1		
С	70	ILE	MET	conflict	UNP A0A7Y1Q2L1		
С	71	GLY	ALA	conflict	UNP A0A7Y1Q2L1		
С	81	MET	ILE	conflict	UNP A0A7Y1Q2L1		
С	85	LEU	PRO	conflict	UNP A0A7Y1Q2L1		
С	88	THR	ALA	conflict	UNP A0A7Y1Q2L1		
С	89	ALA	GLY	conflict	UNP A0A7Y1Q2L1		
С	91	ASP	GLY	conflict	UNP A0A7Y1Q2L1		
С	?	-	GLY	deletion	UNP A0A7Y1Q2L1		
С	93	GLU	ILE	conflict	UNP A0A7Y1Q2L1		
С	99	ASN	SER	conflict	UNP A0A7Y1Q2L1		
С	101	THR	SER	conflict	UNP A0A7Y1Q2L1		
С	201	VAL	TYR	conflict	UNP A0A7Y1Q2L1		
С	314	LEU	VAL	conflict	UNP A0A7Y1Q2L1		
С	363	LYS	ARG	conflict	UNP A0A7Y1Q2L1		
С	370	VAL	ILE	conflict	UNP A0A7Y1Q2L1		
D	-14	TRP	-	expression tag	UNP A0A7Y1Q2L1		
D	-13	SER	-	expression tag	UNP A0A7Y1Q2L1		
D	-12	HIS	-	expression tag	UNP A0A7Y1Q2L1		
D	-11	PRO	-	expression tag	UNP A0A7Y1Q2L1		
D	-10	GLN	-	expression tag	UNP A0A7Y1Q2L1		

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	PHE	-	expression tag	UNP A0A7Y1Q2L1
D	-8	GLU	-	expression tag	UNP A0A7Y1Q2L1
D	-7	LYS	-	expression tag	UNP A0A7Y1Q2L1
D	-6	GLU	-	expression tag	UNP A0A7Y1Q2L1
D	-5	ASN	-	expression tag	UNP A0A7Y1Q2L1
D	-4	LEU	-	expression tag	UNP A0A7Y1Q2L1
D	-3	TYR	-	expression tag	UNP A0A7Y1Q2L1
D	-2	PHE	-	expression tag	UNP A0A7Y1Q2L1
D	-1	GLN	-	expression tag	UNP A0A7Y1Q2L1
D	0	GLY	-	expression tag	UNP A0A7Y1Q2L1
D	3	ARG	GLN	conflict	UNP A0A7Y1Q2L1
D	69	ALA	THR	conflict	UNP A0A7Y1Q2L1
D	70	ILE	MET	conflict	UNP A0A7Y1Q2L1
D	71	GLY	ALA	conflict	UNP A0A7Y1Q2L1
D	81	MET	ILE	conflict	UNP A0A7Y1Q2L1
D	85	LEU	PRO	conflict	UNP A0A7Y1Q2L1
D	88	THR	ALA	conflict	UNP A0A7Y1Q2L1
D	89	ALA	GLY	conflict	UNP A0A7Y1Q2L1
D	91	ASP	GLY	conflict	UNP A0A7Y1Q2L1
D	?	-	GLY	deletion	UNP A0A7Y1Q2L1
D	93	GLU	ILE	conflict	UNP A0A7Y1Q2L1
D	99	ASN	SER	conflict	UNP A0A7Y1Q2L1
D	101	THR	SER	conflict	UNP A0A7Y1Q2L1
D	201	VAL	TYR	conflict	UNP A0A7Y1Q2L1
D	314	LEU	VAL	conflict	UNP A0A7Y1Q2L1
D	363	LYS	ARG	conflict	UNP A0A7Y1Q2L1
D	370	VAL	ILE	conflict	UNP A0A7Y1Q2L1
Е	-14	TRP	-	expression tag	UNP A0A7Y1Q2L1
Е	-13	SER	-	expression tag	UNP A0A7Y1Q2L1
Е	-12	HIS	-	expression tag	UNP A0A7Y1Q2L1
Е	-11	PRO	-	expression tag	UNP A0A7Y1Q2L1
Е	-10	GLN	-	expression tag	UNP A0A7Y1Q2L1
Е	-9	PHE	-	expression tag	UNP A0A7Y1Q2L1
Е	-8	GLU	-	expression tag	UNP A0A7Y1Q2L1
Е	-7	LYS	-	expression tag	UNP A0A7Y1Q2L1
Е	-6	GLU	-	expression tag	UNP A0A7Y1Q2L1
Е	-5	ASN	-	expression tag	UNP A0A7Y1Q2L1
Е	-4	LEU	-	expression tag	UNP A0A7Y1Q2L1
Е	-3	TYR	-	expression tag	UNP A0A7Y1Q2L1
Е	-2	PHE	-	expression tag	UNP A0A7Y1Q2L1
Е	-1	GLN	-	expression tag	UNP A0A7Y1Q2L1
Е	0	GLY	-	expression tag	UNP A0A7Y1Q2L1

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Chain	Residue	Modelled	Actual	Comment	Reference			
E	3	ARG	GLN	conflict	UNP A0A7Y1Q2L1			
E	69	ALA	THR	conflict	UNP A0A7Y1Q2L1			
E	70	ILE	MET	conflict	UNP A0A7Y1Q2L1			
E	71	GLY	ALA	conflict	UNP A0A7Y1Q2L1			
E	81	MET	ILE	conflict	UNP A0A7Y1Q2L1			
E	85	LEU	PRO	conflict	UNP A0A7Y1Q2L1			
E	88	THR	ALA	conflict	UNP A0A7Y1Q2L1			
E	89	ALA	GLY	conflict	UNP A0A7Y1Q2L1			
E	91	ASP	GLY	conflict	UNP A0A7Y1Q2L1			
E	?	-	GLY	deletion	UNP A0A7Y1Q2L1			
E	93	GLU	ILE	conflict	UNP A0A7Y1Q2L1			
E	99	ASN	SER	conflict	UNP A0A7Y1Q2L1			
E	101	THR	SER	conflict	UNP A0A7Y1Q2L1			
Е	201	VAL	TYR	conflict	UNP A0A7Y1Q2L1			
Е	314	LEU	VAL	conflict	UNP A0A7Y1Q2L1			
Е	363	LYS	ARG	conflict	UNP A0A7Y1Q2L1			
Е	370	VAL	ILE	conflict	UNP A0A7Y1Q2L1			
F	-14	TRP	-	expression tag	UNP A0A7Y1Q2L1			
F	-13	SER	-	expression tag	UNP A0A7Y1Q2L1			
F	-12	HIS	-	expression tag	UNP A0A7Y1Q2L1			
F	-11	PRO	-	expression tag	UNP A0A7Y1Q2L1			
F	-10	GLN	-	expression tag	UNP A0A7Y1Q2L1			
F	-9	PHE	-	expression tag	UNP A0A7Y1Q2L1			
F	-8	GLU	-	expression tag	UNP A0A7Y1Q2L1			
F	-7	LYS	-	expression tag	UNP A0A7Y1Q2L1			
F	-6	GLU	-	expression tag	UNP A0A7Y1Q2L1			
F	-5	ASN	-	expression tag	UNP A0A7Y1Q2L1			
F	-4	LEU	-	expression tag	UNP A0A7Y1Q2L1			
F	-3	TYR	-	expression tag	UNP A0A7Y1Q2L1			
F	-2	PHE	-	expression tag	UNP A0A7Y1Q2L1			
F	-1	GLN	-	expression tag	UNP A0A7Y1Q2L1			
F	0	GLY	-	expression tag	UNP A0A7Y1Q2L1			
F	3	ARG	GLN	conflict	UNP A0A7Y1Q2L1			
F	69	ALA	THR	conflict	UNP A0A7Y1Q2L1			
F	70	ILE	MET	conflict	UNP A0A7Y1Q2L1			
F	71	GLY	ALA	conflict	UNP A0A7Y1Q2L1			
F	81	MET	ILE	conflict	UNP A0A7Y1Q2L1			
F	85	LEU	PRO	conflict	UNP A0A7Y1Q2L1			
F	88	THR	ALA	conflict	UNP A0A7Y1Q2L1			
F	89	ALA	GLY	conflict	UNP A0A7Y1Q2L1			
F	91	ASP	GLY	conflict	UNP A0A7Y1Q2L1			
F	?	-	GLY	deletion	UNP A0A7Y1Q2L1			

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Chain	Residue	Modelled	Actual	Comment	Reference
Onam	Itestute	wibuciicu	neuuai	Commente	neicrenee
F	93	GLU	ILE	conflict	UNP A0A7Y1Q2L1
F	99	ASN	SER	conflict	UNP A0A7Y1Q2L1
F	101	THR	SER	conflict	UNP A0A7Y1Q2L1
F	201	VAL	TYR	conflict	UNP A0A7Y1Q2L1
F	314	LEU	VAL	conflict	UNP A0A7Y1Q2L1
F	363	LYS	ARG	conflict	UNP A0A7Y1Q2L1
F	370	VAL	ILE	conflict	UNP A0A7Y1Q2L1

• Molecule 2 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		A	Aton	ıs			ZeroOcc	AltConf				
0	2 1	1	Total	С	Η	Ν	0	Р	0	0				
	1	38	10	11	5	10	2	0	0					
9	В	1	Total	С	Η	Ν	Ο	Р	0	0				
	D	T	38	10	11	5	10	2		0				
9	С	С	C	C	1	Total	С	Η	Ν	Ο	Р	0	0	
		1	38	10	11	5	10	2	0	0				
9	Л	1	Total	С	Η	Ν	Ο	Р	0	0				
	D	1	38	10	11	5	10	2		0				
9	F	F	Г	Б	F	1	Total	С	Η	Ν	Ο	Р	0	0
	1	38	10	11	5	10	2	0	0					
0	Б	1	Total	С	Η	Ν	Ο	Р	0	0				
	Г	1	38	10	11	5	10	2	0	0				

• Molecule 3 is L-METHIONINE-S-SULFOXIMINE PHOSPHATE (three-letter code: P3S) (formula: $C_5H_{13}N_2O_6PS$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues			Atc	ms				ZeroOcc	AltConf								
3	2 1	1	Total	С	Η	Ν	0	Р	S	0	1								
0	A	1	25	5	10	2	6	1	1	0	1								
3	В	1	Total	С	Η	Ν	0	Р	\mathbf{S}	0	1								
0	D		25	5	10	2	6	1	1	0	1								
3	С	С	С	С	С	С	С	С	С	1	Total	С	Η	Ν	0	Р	\mathbf{S}	0	1
0	U	1	25	5	10	2	6	1	1	0	Ţ								
2	Л	D 1	Total	С	Η	Ν	Ο	Р	\mathbf{S}	0	1								
0	D		25	5	10	2	6	1	1	0									
3	Г	Б	Б	Г	Б	Г	1	Total	С	Η	Ν	0	Р	S	0	1			
	1	25	5	10	2	6	1	1	0	1									
2 F	F 1	Total	С	Η	Ν	Ο	Р	S	0	1									
3	Г	1	25	5	10	2	6	1	1	0									

• Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	2	Total Mn 2 2	0	0
4	В	2	Total Mn 2 2	0	0
4	С	2	Total Mn 2 2	0	0
4	D	2	Total Mn 2 2	0	0
4	Е	2	Total Mn 2 2	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	2	Total Mn 2 2	0	0

• Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total Mg 1 1	0	0
5	В	1	Total Mg 1 1	0	0
5	С	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0
5	Е	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	103	Total O 103 103	0	0
6	В	107	Total O 107 107	0	0
6	С	110	Total O 110 110	0	0
6	D	111	Total O 111 111	0	0
6	Е	120	Total O 120 120	0	0
6	F	106	Total O 106 106	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: Glutamine synthetase



E164 E164

G385 V394 L403 R409 R415 M457 M457 M457 M457 M455 M474 M455 M474 M456 M456

 \bullet Molecule 1: Glutamine synthetase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	123.06Å 140.48Å 216.66Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	43.77 - 2.30	Depositor
	46.84 - 2.30	EDS
% Data completeness	99.8 (43.77-2.30)	Depositor
(in resolution range)	$100.0 \ (46.84 - 2.30)$	EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.71 (at 2.29 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.20.1_4487: 000)	Depositor
B B.	0.212 , 0.232	Depositor
n, n_{free}	0.211 , 0.232	DCC
R_{free} test set	8314 reflections $(4.99%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	35.3	Xtriage
Anisotropy	0.846	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.39, 38.1	EDS
L-test for twinning ²	$ L > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	46408	wwPDB-VP
Average B, all atoms $(Å^2)$	54.0	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 40.08 % 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 2.8856e-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: P3S, ADP, MG, MN

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	$RMSZ \mid \# Z > 5$		RMSZ	# Z > 5	
1	А	0.39	0/3922	0.67	0/5322	
1	В	0.40	0/3912	0.64	0/5307	
1	С	0.38	0/3922	0.64	0/5322	
1	D	0.43	0/3922	0.68	0/5322	
1	Е	0.39	0/3913	0.67	0/5308	
1	F	0.36	0/3922	0.62	0/5322	
All	All	0.39	0/23513	0.65	0/31903	

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	3828	3737	3755	24	0
1	В	3819	3705	3746	34	0
1	С	3828	3732	3755	27	0
1	D	3828	3724	3755	23	0
1	Е	3820	3751	3750	20	0
1	F	3828	3755	3755	35	0
2	А	27	11	12	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	27	11	12	0	0
2	С	27	11	12	0	0
2	D	27	11	12	0	0
2	Е	27	11	12	1	0
2	F	27	11	12	0	0
3	А	15	10	0	0	0
3	В	15	10	0	0	0
3	С	15	10	0	0	0
3	D	15	10	0	0	0
3	Е	15	10	0	0	0
3	F	15	10	0	0	0
4	А	2	0	0	0	0
4	В	2	0	0	0	0
4	С	2	0	0	0	0
4	D	2	0	0	0	0
4	Е	2	0	0	0	0
4	F	2	0	0	0	0
5	А	1	0	0	0	0
5	В	1	0	0	0	0
5	С	1	0	0	0	0
5	D	1	0	0	0	0
5	Е	1	0	0	0	0
5	F	1	0	0	0	0
6	А	103	0	0	1	0
6	В	107	0	0	0	0
6	С	110	0	0	1	0
6	D	111	0	0	0	0
6	Е	120	0	0	0	0
6	F	106	0	0	1	0
All	All	23878	22530	22588	158	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.

All (158) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-1 Atom-2		Clash overlap (Å)	
1:F:36:MET:HE1	1:F:54:THR:HG22	1.51	0.93	
1:F:298:ASP:HB3	1:F:301:THR:HG22	1.52	0.91	
1:E:8:ILE:CD1	1:E:105:VAL:HG13	2.15	0.76	
1:A:355:ARG:NH1	1:A:426:MET:SD	2.59	0.74	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:367:VAL:HG13	1:A:380:ILE:HG23	1.70	0.72	
1:C:313:VAL:HG11	1:C:415:LEU:HD11	1.71	0.72	
1:C:367:VAL:HG13	1:C:380:ILE:HG23	1.71	0.71	
1:B:51:LYS:HE3	1:B:68:VAL:HG12	1.73	0.70	
1:F:298:ASP:CB	1:F:301:THR:HG22	2.21	0.70	
1:D:367:VAL:HG13	1:D:380:ILE:HG23	1.74	0.70	
1:E:8:ILE:HD12	1:E:105:VAL:HG13	1.73	0.69	
1:F:310:GLU:HA	1:F:373:THR:HG21	1.75	0.69	
1:F:36:MET:HE2	1:F:54:THR:HA	1.74	0.68	
1:B:39:LEU:HD23	1:B:104:MET:HE2	1.75	0.67	
1:C:151:SER:OG	1:C:299:LYS:HE2	1.95	0.67	
1:B:367:VAL:HG13	1:B:380:ILE:HG23	1.77	0.65	
1:A:357:ALA:HB2	1:A:424:VAL:HG21	1.78	0.65	
1:F:148:LYS:NZ	1:F:152:ASP:OD1	2.26	0.65	
1:B:87:THR:HG23	1:B:87:THR:O	1.98	0.63	
1:F:36:MET:CE	1:F:54:THR:HG22	2.26	0.63	
1:E:39:LEU:HD23	1:E:104:MET:HE3	1.81	0.62	
1:D:39:LEU:HD21	1:D:106:PRO:HG3	1.80	0.62	
1:E:367:VAL:HG13	1:E:380:ILE:HG23	1.81	0.62	
1:C:78:VAL:CG1	1:C:78:VAL:O	2.47	0.62	
1:C:145:LYS:O	1:C:148:LYS:HG3	2.03	0.59	
1:C:161:ILE:HD12	1:C:247:MET:CE	2.34	0.58	
1:F:297:VAL:CG1	1:F:302:ARG:HA	2.34	0.58	
1:B:39:LEU:HD12	1:B:123:MET:HG2	1.86	0.58	
1:F:367:VAL:HG13	1:F:380:ILE:HG23	1.85	0.57	
1:A:326:LEU:O	1:A:356:ARG:HD2	2.04	0.56	
1:C:78:VAL:O	1:C:78:VAL:HG12	2.04	0.56	
1:F:326:LEU:HD11	1:F:358:TRP:HB3	1.86	0.56	
1:C:88:THR:HB	1:F:417:GLU:HG3	1.87	0.55	
1:B:78:VAL:HG11	1:B:186:GLN:HG2	1.89	0.54	
1:E:357:ALA:HB2	1:E:424:VAL:HG21	1.89	0.54	
1:F:58:LEU:HD11	1:F:123:MET:HE1	1.89	0.54	
1:B:436:ASP:OD1	1:B:462:ARG:NH2	2.41	0.54	
1:F:6:ASP:O	1:F:10:LYS:HD3	2.08	0.54	
1:D:353:PRO:HB3	1:D:366:MET:HA	1.89	0.54	
1:C:360:LYS:NZ	1:C:371:SER:O	2.36	0.53	
1:A:227:PRO:HB2	1:A:245:ASP:HB2	1.91	0.53	
1:D:180:LEU:HD11	1:E:194:PRO:HG2	1.90	0.53	
1:D:234:GLU:HG3	1:D:235:TRP:H	1.74	0.52	
1:F:212:ASP:N	1:F:212:ASP:OD1	2.41	0.52	
1:E:55:VAL:O	1:E:59:LYS:HG2	2.09	0.52	



	lo uo pugom	Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:E:475:GLU:HG2	1:E:476:ALA:N	2.24	0.52		
1:D:475:GLU:HG2	1:D:476:ALA:N	2.25	0.52		
1:E:313:VAL:HG11	1:E:415:LEU:HD11	1.91	0.52		
1:F:357:ALA:HB2	1:F:424:VAL:HG21	1.91	0.52		
1:B:39:LEU:HD23	1:B:104:MET:CE	2.41	0.51		
1:A:326:LEU:HD11	1:A:358:TRP:HB3	1.92	0.51		
1:E:48:LEU:HD21	1:E:257:LEU:HD21	1.93	0.51		
1:F:297:VAL:HG13	1:F:302:ARG:HA	1.93	0.50		
1:C:212:ASP:N	1:C:212:ASP:OD1	2.45	0.50		
1:D:21:ALA:O	1:D:25:VAL:HG23	2.12	0.50		
1:F:457:TRP:O	1:F:461:ARG:HG2	2.11	0.50		
1:D:68:VAL:HG22	1:D:69:ALA:N	2.27	0.49		
1:A:49:ARG:HD2	1:A:72:PRO:HB3	1.95	0.49		
1:E:201:VAL:HG22	1:E:202:LEU:HG	1.95	0.49		
1:B:212:ASP:N	1:B:212:ASP:OD1	2.45	0.49		
1:C:358:TRP:CE2	1:C:415:LEU:HD23	2.48	0.49		
1:D:211:ASP:HA	1:D:214:MET:HB2	1.95	0.48		
1:A:212:ASP:OD1	1:A:212:ASP:N	2.43	0.48		
1:C:457:TRP:O	1:C:461:ARG:HG2	2.14	0.48		
1:A:457:TRP:O	1:A:461:ARG:HG2	2.14	0.47		
1:E:39:LEU:HD21	1:E:106:PRO:HG3	1.96	0.47		
1:A:229:ARG:HG3	1:E:57:SER:OG	2.13	0.47		
1:B:93:GLU:HB3	1:B:452:THR:HG21	1.96	0.47		
1:C:85:LEU:HD23	1:C:98:GLY:O	2.15	0.47		
1:E:212:ASP:OD1	1:E:212:ASP:N	2.47	0.47		
1:E:313:VAL:HG11	1:E:415:LEU:CD1	2.45	0.47		
1:F:186:GLN:HG3	6:F:659:HOH:O	2.15	0.47		
1:D:364:ALA:HB1	1:D:420:TYR:CE2	2.51	0.46		
1:F:445:PHE:O	1:F:449:PHE:HB2	2.17	0.45		
1:A:156:LEU:HB2	1:A:297:VAL:CG2	2.47	0.45		
1:C:78:VAL:HG13	6:C:644:HOH:O	2.15	0.45		
1:A:201:VAL:HG22	1:A:202:LEU:HG	1.97	0.45		
1:D:78:VAL:HG11	1:D:186:GLN:HG2	1.98	0.45		
1:D:348:PRO:O	1:D:420:TYR:CG	2.69	0.45		
1:A:290:TRP:HB2	1:A:387:PRO:HA	1.98	0.45		
1:B:410:LYS:HG3	1:B:411:ASP:N	2.32	0.45		
1:D:9:THR:HG22	1:D:19:ARG:NH2	2.31	0.45		
1:D:432:ALA:HB2	1:D:465:TRP:CE2	2.51	0.45		
1:F:414:GLU:HG3	1:F:416:GLN:NE2	2.32	0.44		
1:D:457:TRP:O	1:D:461:ARG:HG2	2.17	0.44		
1:A:236:ALA:HB3	1:A:239:GLN:HB2	2.00	0.44		



	loub page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:F:49:ARG:HD2	1:F:72:PRO:HB3	2.00	0.44	
1:F:465:TRP:NE1	1:F:469:LEU:HD12	2.32	0.44	
1:E:160:GLY:HA3	2:E:501:ADP:H1'	1.98	0.44	
1:B:87:THR:O	1:B:87:THR:CG2	2.65	0.44	
1:B:457:TRP:O	1:B:461:ARG:HG2	2.18	0.44	
1:F:211:ASP:HA	1:F:214:MET:HB2	2.00	0.43	
1:B:319:ARG:HG3	1:B:358:TRP:CH2	2.53	0.43	
1:B:236:ALA:HB3	1:B:239:GLN:HB2	2.01	0.43	
1:D:135:PHE:CD1	1:D:136:PRO:HD2	2.53	0.43	
1:A:180:LEU:HD11	1:C:194:PRO:HG2	2.00	0.43	
1:C:78:VAL:HG21	1:C:186:GLN:HG2	2.00	0.43	
1:D:106:PRO:HB3	1:D:123:MET:CE	2.49	0.43	
1:F:8:ILE:HG12	1:F:105:VAL:HG13	2.01	0.43	
1:F:326:LEU:O	1:F:356:ARG:HD2	2.18	0.43	
1:C:236:ALA:HB3	1:C:239:GLN:HB2	2.01	0.43	
1:E:18:GLN:O	1:E:108:PRO:HG2	2.18	0.43	
1:B:39:LEU:HB3	1:B:104:MET:HE1	1.99	0.43	
1:A:153:GLU:HG3	1:A:403:LEU:HD11	1.99	0.43	
1:A:432:ALA:HB2	1:A:465:TRP:CE2	2.53	0.43	
1:B:201:VAL:HG22	1:B:202:LEU:HG	1.99	0.43	
1:D:357:ALA:HB2	1:D:424:VAL:HG21	2.00	0.43	
1:C:336:THR:HG22	1:C:394:TYR:CD1	2.54	0.43	
1:E:153:GLU:HG3	1:E:403:LEU:HD11	2.00	0.43	
1:F:290:TRP:HB2	1:F:387:PRO:HA	2.01	0.42	
1:F:364:ALA:HB1	1:F:420:TYR:CE2	2.53	0.42	
1:B:394:TYR:O	1:B:398:GLN:HG2	2.18	0.42	
1:C:201:VAL:HG22	1:C:202:LEU:HG	2.00	0.42	
1:F:35:GLU:O	1:F:36:MET:HE3	2.19	0.42	
1:B:410:LYS:HG3	1:B:411:ASP:H	1.85	0.42	
1:C:179:SER:HB3	1:C:188:ASP:HB2	2.01	0.42	
1:F:308:PRO:HB3	1:F:314:LEU:CA	2.49	0.42	
1:D:150:LEU:HD12	1:D:403:LEU:HD13	2.01	0.42	
1:B:101:THR:HB	1:B:130:LYS:CE	2.50	0.42	
1:D:68:VAL:HG22	1:D:69:ALA:O	2.20	0.42	
1:A:409:LYS:HE3	1:A:409:LYS:HA	2.02	0.41	
1:B:135:PHE:HA	1:B:136:PRO:HD3	1.96	0.41	
1:B:432:ALA:HB2	1:B:465:TRP:CE2	2.55	0.41	
1:C:385:GLY:HA3	1:C:394:TYR:CZ	2.55	0.41	
1:F:39:LEU:CD1	1:F:123:MET:HE3	2.50	0.41	
1:B:40:SER:O	1:B:124:LEU:HA	2.20	0.41	
1:E:353:PRO:HB3	1:E:366:MET:HA	2.02	0.41	



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:153:GLU:HA	1:A:153:GLU:OE1	2.21	0.41	
1:A:199:TYR:OH	1:A:284:GLY:O	2.29	0.41	
1:B:12:ASN:O	1:B:12:ASN:CG	2.58	0.41	
1:C:211:ASP:HA	1:C:214:MET:HB2	2.03	0.41	
1:C:432:ALA:HB2	1:C:465:TRP:CE2	2.56	0.41	
1:B:287:ALA:HB1	1:B:345:ARG:HG3	2.03	0.41	
1:B:345:ARG:HE	1:B:352:ALA:HB2	1.86	0.41	
1:C:156:LEU:HB2	1:C:297:VAL:HG22	2.02	0.41	
1:F:60:SER:O	1:F:64:GLU:HG3	2.21	0.41	
1:F:325:LEU:HD23	1:F:401:SER:HB2	2.03	0.41	
1:F:385:GLY:HA3	1:F:394:TYR:CZ	2.56	0.41	
1:C:158:LYS:O	1:C:294:GLN:HA	2.22	0.41	
1:E:457:TRP:O	1:E:461:ARG:HG2	2.20	0.41	
1:A:211:ASP:HA	1:A:214:MET:HB2	2.03	0.40	
1:B:183:PRO:CG	1:D:286:PHE:HE2	2.35	0.40	
1:D:68:VAL:CG2	1:D:69:ALA:N	2.84	0.40	
1:A:193:GLN:HG2	6:A:686:HOH:O	2.20	0.40	
1:A:319:ARG:HG3	1:A:358:TRP:CH2	2.57	0.40	
1:B:290:TRP:CD1	1:B:290:TRP:C	2.94	0.40	
1:D:445:PHE:O	1:D:449:PHE:HB2	2.21	0.40	
1:F:297:VAL:CG1	1:F:298:ASP:N	2.84	0.40	
1:B:82:VAL:HG21	1:B:460:LEU:HD12	2.03	0.40	

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	488/510~(96%)	486 (100%)	2(0%)	0	100	100
1	В	484/510~(95%)	481 (99%)	3~(1%)	0	100	100
1	С	488/510~(96%)	485 (99%)	3~(1%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	D	488/510~(96%)	485 (99%)	3~(1%)	0	100	100
1	Ε	485/510~(95%)	481 (99%)	4 (1%)	0	100	100
1	F	488/510~(96%)	485 (99%)	3 (1%)	0	100	100
All	All	2921/3060~(96%)	2903 (99%)	18 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	Perce	ntiles
1	А	408/427~(96%)	399~(98%)	9~(2%)	52	69
1	В	408/427~(96%)	402 (98%)	6(2%)	65	79
1	С	408/427~(96%)	400 (98%)	8 (2%)	55	72
1	D	408/427~(96%)	405 (99%)	3~(1%)	84	92
1	Е	407/427~(95%)	402 (99%)	5 (1%)	71	84
1	F	408/427~(96%)	402 (98%)	6(2%)	65	79
All	All	2447/2562~(96%)	2410 (98%)	37~(2%)	65	79

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	64	GLU
1	А	88	THR
1	А	212	ASP
1	А	292	MET
1	А	301	THR
1	А	358	TRP
1	А	373	THR
1	А	417	GLU
1	А	462	ARG
1	В	20	ASP



Mol	Chain	Res	Type
1	В	80	SER
1	В	95	GLU
1	В	292	MET
1	В	301	THR
1	В	358	TRP
1	С	79	SER
1	С	80	SER
1	С	209	GLN
1	С	301	THR
1	С	358	TRP
1	С	373	THR
1	С	409	LYS
1	С	451	ASP
1	D	151	SER
1	D	292	MET
1	D	358	TRP
1	Е	64	GLU
1	Е	66	SER
1	Е	339	THR
1	Е	358	TRP
1	Е	386	GLU
1	F	64	GLU
1	F	123	MET
1	F	153	GLU
1	F	212	ASP
1	F	358	TRP
1	F	469	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	408	ASN
1	Е	191	GLN
1	F	84	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.



5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 18 are monoatomic - leaving 18 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).

Mal	Turne	Chain	Deg Link		Bond lengths		Bond angles			
INIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	ADP	D	501	4,5	24,29,29	0.91	2 (8%)	$29,\!45,\!45$	1.51	4 (13%)
2	ADP	С	501	4,5	$24,\!29,\!29$	0.93	2 (8%)	$29,\!45,\!45$	1.58	5 (17%)
2	ADP	В	501	4,5	$24,\!29,\!29$	0.95	2 (8%)	$29,\!45,\!45$	1.52	4 (13%)
2	ADP	Е	501	4,5	24,29,29	0.97	2 (8%)	$29,\!45,\!45$	1.56	4 (13%)
2	ADP	F	501	4,5	24,29,29	0.93	2 (8%)	29,45,45	1.50	5 (17%)
2	ADP	А	501	4,5	24,29,29	0.93	2 (8%)	29,45,45	1.50	5 (17%)

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
2	ADP	D	501	4,5	-	2/12/32/32	0/3/3/3
2	ADP	С	501	4,5	-	1/12/32/32	0/3/3/3
2	ADP	В	501	4,5	-	3/12/32/32	0/3/3/3
2	ADP	Е	501	4,5	-	2/12/32/32	0/3/3/3
2	ADP	F	501	4,5	-	4/12/32/32	0/3/3/3
2	ADP	А	501	4,5	-	1/12/32/32	0/3/3/3



8	W	W	V
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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Е	501	ADP	O4'-C1'	2.49	1.44	1.41
2	В	501	ADP	O4'-C1'	2.42	1.44	1.41
2	А	501	ADP	O4'-C1'	2.39	1.44	1.41
2	С	501	ADP	O4'-C1'	2.35	1.44	1.41
2	F	501	ADP	O4'-C1'	2.31	1.44	1.41
2	Е	501	ADP	C5-C4	2.12	1.46	1.40
2	F	501	ADP	C5-C4	2.08	1.46	1.40
2	А	501	ADP	C5-C4	2.08	1.46	1.40
2	С	501	ADP	C5-C4	2.08	1.46	1.40
2	В	501	ADP	C5-C4	2.08	1.46	1.40
2	D	501	ADP	O4'-C1'	2.07	1.44	1.41
2	D	501	ADP	C5-C4	2.04	1.46	1.40

All (12) bond length outliers are listed below:

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Е	501	ADP	C1'-N9-C4	-4.13	119.39	126.64
2	С	501	ADP	N3-C2-N1	-4.11	122.25	128.68
2	F	501	ADP	N3-C2-N1	-4.06	122.34	128.68
2	А	501	ADP	N3-C2-N1	-4.02	122.40	128.68
2	В	501	ADP	N3-C2-N1	-4.01	122.42	128.68
2	D	501	ADP	N3-C2-N1	-3.98	122.46	128.68
2	Е	501	ADP	N3-C2-N1	-3.98	122.46	128.68
2	С	501	ADP	C1'-N9-C4	-3.82	119.92	126.64
2	F	501	ADP	C1'-N9-C4	-3.82	119.93	126.64
2	D	501	ADP	C1'-N9-C4	-3.63	120.26	126.64
2	В	501	ADP	C1'-N9-C4	-3.31	120.83	126.64
2	Е	501	ADP	C4-C5-N7	-3.28	105.98	109.40
2	В	501	ADP	C4-C5-N7	-3.26	106.00	109.40
2	С	501	ADP	C4-C5-N7	-3.13	106.13	109.40
2	D	501	ADP	C4-C5-N7	-3.11	106.16	109.40
2	F	501	ADP	C4-C5-N7	-3.09	106.18	109.40
2	В	501	ADP	PA-O3A-PB	-2.97	122.64	132.83
2	А	501	ADP	C4-C5-N7	-2.95	106.33	109.40
2	А	501	ADP	C1'-N9-C4	-2.92	121.51	126.64
2	А	501	ADP	PA-O3A-PB	-2.78	123.28	132.83
2	Е	501	ADP	PA-O3A-PB	-2.69	123.59	132.83
2	С	501	ADP	PA-O3A-PB	-2.48	124.32	132.83
2	D	501	ADP	PA-O3A-PB	-2.39	124.61	132.83
2	F	501	ADP	PA-O3A-PB	-2.31	124.90	132.83
2	С	501	ADP	C2-N1-C6	2.19	122.50	118.75
2	А	501	ADP	C2-N1-C6	2.10	122.34	118.75



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	F	501	ADP	C2-N1-C6	2.04	122.24	118.75

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	501	ADP	PA-O3A-PB-O3B
2	F	501	ADP	O4'-C4'-C5'-O5'
2	D	501	ADP	O4'-C4'-C5'-O5'
2	С	501	ADP	O4'-C4'-C5'-O5'
2	В	501	ADP	O4'-C4'-C5'-O5'
2	Е	501	ADP	PA-O3A-PB-O2B
2	Ε	501	ADP	O4'-C4'-C5'-O5'
2	А	501	ADP	O4'-C4'-C5'-O5'
2	F	501	ADP	C3'-C4'-C5'-O5'
2	F	501	ADP	PA-O3A-PB-O1B
2	D	501	ADP	PA-O3A-PB-O2B
2	В	501	ADP	PB-O3A-PA-O2A
2	В	501	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Е	501	ADP	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 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	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	490/510~(96%)	0.60	46 (9%) 8 11	30, 48, 81, 105	0
1	В	488/510~(95%)	0.59	47 (9%) 8 10	29, 48, 79, 104	0
1	С	490/510~(96%)	0.43	27 (5%) 25 31	31, 47, 75, 95	0
1	D	490/510~(96%)	0.32	16 (3%) 46 53	30, 46, 70, 87	0
1	Ε	489/510~(95%)	0.28	22 (4%) 33 40	29, 44, 71, 98	0
1	F	490/510~(96%)	0.36	29 (5%) 22 28	30, 45, 75, 98	0
All	All	2937/3060~(95%)	0.43	187 (6%) 19 25	29, 47, 76, 105	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	92	PHE	7.4
1	А	420	TYR	7.0
1	В	92	PHE	4.7
1	В	420	TYR	4.6
1	А	89	ALA	4.5
1	Е	423	GLN	4.5
1	F	423	GLN	4.4
1	А	372	ALA	4.3
1	D	351	LEU	4.1
1	F	91	ASP	4.0
1	А	87	THR	4.0
1	С	148	LYS	4.0
1	А	423	GLN	4.0
1	В	469	LEU	3.9
1	С	302	ARG	3.8
1	A	309	SER	3.8
1	А	469	LEU	3.8
1	В	423	GLN	3.8
1	В	357	ALA	3.7



Mol	Chain	Res	Type	RSRZ
1	А	424	VAL	3.7
1	А	13	LEU	3.6
1	А	310	GLU	3.5
1	А	12	ASN	3.4
1	D	475	GLU	3.3
1	F	309	SER	3.3
1	В	349	TYR	3.3
1	Е	278	CYS	3.3
1	А	64	GLU	3.3
1	С	372	ALA	3.3
1	В	302	ARG	3.3
1	Е	12	ASN	3.2
1	А	421	ASP	3.2
1	F	87	THR	3.2
1	F	373	THR	3.2
1	С	310	GLU	3.2
1	Е	310	GLU	3.2
1	В	417	GLU	3.1
1	В	309	SER	3.1
1	А	419	PRO	3.1
1	В	13	LEU	3.1
1	В	471	ALA	3.1
1	Е	88	THR	3.1
1	F	9	THR	3.1
1	В	91	ASP	3.1
1	Е	24	LYS	3.1
1	Е	94	ASP	3.0
1	В	475	GLU	3.0
1	В	313	VAL	3.0
1	С	371	SER	3.0
1	В	310	GLU	3.0
1	В	138	CYS	3.0
1	А	301	THR	3.0
1	С	300	ASP	2.9
1	F	8	ILE	2.9
1	D	310	GLU	2.9
1	А	163	LEU	2.9
1	С	374	GLY	2.9
1	А	256	ALA	2.9
1	Е	309	SER	2.9
1	А	290	TRP	2.9
1	F	94	ASP	2.9



Mol	Chain	Res	Type	RSRZ
1	В	130	LYS	2.9
1	D	12	ASN	2.8
1	F	16	ASN	2.8
1	F	13	LEU	2.8
1	А	311	GLY	2.8
1	В	16	ASN	2.8
1	В	424	VAL	2.8
1	С	474	ALA	2.8
1	D	27	ALA	2.8
1	В	10	LYS	2.8
1	А	414	GLU	2.8
1	В	20	ASP	2.8
1	В	311	GLY	2.7
1	С	475	GLU	2.7
1	С	12	ASN	2.7
1	Е	13	LEU	2.7
1	В	9	THR	2.7
1	В	12	ASN	2.7
1	А	391	PRO	2.7
1	Е	87	THR	2.7
1	С	131	SER	2.7
1	D	89	ALA	2.7
1	В	421	ASP	2.7
1	А	393	LEU	2.7
1	D	17	GLU	2.6
1	А	21	ALA	2.6
1	А	276	PHE	2.6
1	Е	163	LEU	2.6
1	А	95	GLU	2.6
1	А	349	TYR	2.6
1	С	313	VAL	2.6
1	F	424	VAL	2.6
1	Е	89	ALA	2.6
1	F	372	ALA	2.6
1	С	309	SER	2.6
1	F	475	GLU	2.5
1	А	440	HIS	2.5
1	F	90	GLY	2.5
1	А	474	ALA	2.5
1	F	89	ALA	2.5
1	Е	8	ILE	2.5
1	В	95	GLU	2.5



Mol	Chain	Res	Type	RSRZ
1	В	290	TRP	2.5
1	В	7	PHE	2.5
1	В	8	ILE	2.5
1	С	311	GLY	2.5
1	D	469	LEU	2.5
1	D	69	ALA	2.5
1	В	87	THR	2.5
1	С	79	SER	2.4
1	А	16	ASN	2.4
1	Е	133	GLU	2.4
1	Е	242	THR	2.4
1	А	373	THR	2.4
1	Е	475	GLU	2.4
1	Е	10	LYS	2.4
1	С	403	LEU	2.4
1	F	203	LEU	2.4
1	С	154	GLY	2.4
1	А	395	MET	2.4
1	Е	17	GLU	2.4
1	А	300	ASP	2.4
1	А	88	THR	2.4
1	А	242	THR	2.4
1	В	17	GLU	2.4
1	Е	290	TRP	2.3
1	D	302	ARG	2.3
1	F	10	LYS	2.3
1	F	302	ARG	2.3
1	В	96	LEU	2.3
1	В	252	ALA	2.3
1	В	88	THR	2.3
1	F	300	ASP	2.3
1	А	313	VAL	2.3
1	А	138	CYS	2.3
1	С	20	ASP	2.3
1	А	418	SER	2.3
1	F	92	PHE	2.3
1	D	42	ALA	2.3
1	С	9	THR	2.2
1	А	394	TYR	2.2
1	В	426	MET	2.2
1	F	310	GLU	2.2
1	В	355	ARG	2.2



Mol	Chain	Res	Type	RSRZ	
1	В	474	ALA	2.2	
1	С	324	GLY	2.2	
1	В	165	TRP	2.2	
1	В	473	GLY	2.2	
1	С	8	ILE	2.2	
1	F	163	LEU	2.2	
1	В	422	ALA	2.2	
1	Е	243	THR	2.2	
1	С	47	LEU	2.2	
1	С	48	LEU	2.2	
1	В	395	MET	2.2	
1	Е	92	PHE	2.2	
1	F	7	PHE	2.2	
1	D	138	CYS	2.2	
1	F	17	GLU	2.2	
1	А	139	PRO	2.2	
1	Е	421	ASP	2.2	
1	С	27	ALA	2.1	
1	А	161	ILE	2.1	
1	D	20	ASP	2.1	
1	D	163	LEU	2.1	
1	D	16	ASN	2.1	
1	С	320	ALA	2.1	
1	А	308	PRO	2.1	
1	D	309	SER	2.1	
1	В	396	ALA	2.1	
1	F	88	THR	2.1	
1	F	308	PRO	2.1	
1	F	12	ASN	2.1	
1	С	370	VAL	2.1	
1	А	46	GLY	2.1	
1	В	289	GLY	2.1	
1	F	417	GLU	2.0	
1	В	300	ASP	2.0	
1	А	8	ILE	2.0	
1	А	422	ALA	2.0	
1	В	412	PRO	2.0	
1	F	307	ILE	2.0	
1	С	417	GLU	2.0	
1	В	163	LEU	2.0	
1	А	388	GLY	2.0	
1	В	27	ALA	2.0	

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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
5	MG	С	505	1/1	0.57	0.19	64,64,64,64	0
5	MG	А	505	1/1	0.58	0.34	53,53,53,53	0
5	MG	D	505	1/1	0.65	0.23	55,55,55,55	0
4	MN	С	503	1/1	0.79	0.09	59,59,59,59	0
3	P3S	С	502[A]	15/15	0.82	0.25	52,79,95,103	1
3	P3S	С	502[B]	15/15	0.82	0.25	52,79,95,103	1
5	MG	В	505	1/1	0.83	0.39	54,54,54,54	0
4	MN	D	504	1/1	0.83	0.13	79,79,79,79	0
4	MN	С	504	1/1	0.83	0.11	85,85,85,85	0
5	MG	Е	505	1/1	0.83	0.21	41,41,41,41	0
3	P3S	В	502[A]	15/15	0.84	0.22	54,72,80,81	1
3	P3S	В	502[B]	15/15	0.84	0.22	54,72,80,81	1
5	MG	F	505	1/1	0.85	0.27	45,45,45,45	0
3	P3S	D	502[B]	15/15	0.89	0.18	47,72,83,88	1
3	P3S	D	502[A]	15/15	0.89	0.18	47,72,83,88	1
4	MN	А	504	1/1	0.90	0.05	$65,\!65,\!65,\!65$	0
4	MN	В	504	1/1	0.91	0.09	80,80,80,80	0
4	MN	F	504	1/1	0.91	0.07	63,63,63,63	0
2	ADP	С	501	27/27	0.92	0.14	47,56,68,72	0
3	P3S	А	502[A]	15/15	0.92	0.14	50,63,73,77	1
3	P3S	А	502[B]	15/15	0.92	0.14	50,63,73,77	1
3	P3S	F	502[B]	15/15	0.93	0.21	43,52,55,56	1
2	ADP	А	501	27/27	0.93	0.15	40,49,59,63	0
4	MN	Е	504	1/1	0.93	0.13	59,59,59,59	0
2	ADP	D	501	27/27	0.93	0.14	41,50,56,57	0
3	P3S	F	502[A]	15/15	0.93	0.21	43,52,55,56	1
2	ADP	F	501	27/27	0.94	0.17	41,45,56,58	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
2	ADP	В	501	27/27	0.94	0.16	42,51,60,62	0
4	MN	D	503	1/1	0.95	0.07	50,50,50,50	0
2	ADP	Е	501	27/27	0.95	0.16	38,44,55,56	0
4	MN	F	503	1/1	0.96	0.06	47,47,47,47	0
4	MN	Е	503	1/1	0.96	0.03	61,61,61,61	0
3	P3S	Е	502[A]	15/15	0.97	0.12	41,44,52,52	1
3	P3S	Е	502[B]	15/15	0.97	0.12	41,44,52,52	1
4	MN	В	503	1/1	0.98	0.08	54,54,54,54	0
4	MN	А	503	1/1	0.98	0.04	54,54,54,54	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.

