

wwPDB X-ray Structure Validation Summary Report (i)

Aug 21, 2021 – 12:26 PM EDT

PDB ID	:	7MFO
Title	:	X-ray structure of the L136 Aminotransferase from Acanthamoeba polyphaga
		mimivirus in the presence of TDP and PMP
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Deposited on	:	2021-04-10
Resolution	:	1.70 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 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	:	2.23.1
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)	:	2.23.1

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	356	89%	9%	·
1	В	356	2% 91%	7%	•
1	С	356	3% 92%	7%	, •
1	D	356	90%	8%	
1	Е	356	2% 92%	7%	, •



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Mol	Chain	Length	Quality of chain		
1	F	356	3% 92%	6%	•
1	G	356	88%	10%	•
1	Н	356	4% 92%	5%	••
1	Ι	356	83%	15%	••
1	J	356	3% 	10%	••

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	TYD	В	403	-	-	Х	-
6	TYD	Е	402	-	-	Х	-
6	TYD	Е	403	-	-	Х	-



$7 \mathrm{MFO}$

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 31417 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	348	Total	С	Ν	0	S	0	0	0
1	Л	040	2783	1780	470	522	11	0	0	0
1	В	350	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	2	0
	D	550	2810	1802	472	525	11	0		0
1	С	352	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	2	0
	0	552	2811	1799	474	527	11	0		0
1	Л	351	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	1	0
	D		2808	1799	473	525	11	0	T	0
1	E	353	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	1	0
-		000	2831	1812	478	529	12	0	1	0
1	F	350	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	1	0
	1	330	2801	1792	473	525	11	0	1	0
1	G	352	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
1	ŭ	002	2809	1797	475	526	11	0	0	0
1	н	351	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	1	0
1	11	001	2801	1794	473	523	11	0	1	0
1	т	350	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
	L	550	2792	1787	472	522	11		0	0
1	T	351	Total	\mathbf{C}	N	0	S	0	1	0
L	J	001	2809	1799	474	525	11	0	1	

• Molecule 1 is a protein called L136 aminotransferase.

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-3	GLY	-	expression tag	UNP Q5UPL1
А	-2	GLY	-	expression tag	UNP Q5UPL1
А	-1	GLY	-	expression tag	UNP Q5UPL1
А	0	HIS	-	expression tag	UNP Q5UPL1
В	-3	GLY	-	expression tag	UNP Q5UPL1
В	-2	GLY	-	expression tag	UNP Q5UPL1
В	-1	GLY	-	expression tag	UNP Q5UPL1
В	0	HIS	-	expression tag	UNP Q5UPL1
С	-3	GLY	-	expression tag	UNP Q5UPL1



Chain	Residue	Modelled	Actual	Comment	Reference
С	-2	GLY	-	expression tag	UNP Q5UPL1
С	-1	GLY	-	expression tag	UNP Q5UPL1
С	0	HIS	-	expression tag	UNP Q5UPL1
D	-3	GLY	-	expression tag	UNP Q5UPL1
D	-2	GLY	-	expression tag	UNP Q5UPL1
D	-1	GLY	-	expression tag	UNP Q5UPL1
D	0	HIS	-	expression tag	UNP Q5UPL1
Е	-3	GLY	-	expression tag	UNP Q5UPL1
Е	-2	GLY	-	expression tag	UNP Q5UPL1
Е	-1	GLY	-	expression tag	UNP Q5UPL1
Е	0	HIS	-	expression tag	UNP Q5UPL1
F	-3	GLY	-	expression tag	UNP Q5UPL1
F	-2	GLY	-	expression tag	UNP Q5UPL1
F	-1	GLY	-	expression tag	UNP Q5UPL1
F	0	HIS	-	expression tag	UNP Q5UPL1
G	-3	GLY	-	expression tag	UNP Q5UPL1
G	-2	GLY	-	expression tag	UNP Q5UPL1
G	-1	GLY	-	expression tag	UNP Q5UPL1
G	0	HIS	-	expression tag	UNP Q5UPL1
Н	-3	GLY	-	expression tag	UNP Q5UPL1
Н	-2	GLY	-	expression tag	UNP Q5UPL1
Н	-1	GLY	-	expression tag	UNP Q5UPL1
Н	0	HIS	-	expression tag	UNP Q5UPL1
Ι	-3	GLY	-	expression tag	UNP Q5UPL1
Ι	-2	GLY	-	expression tag	UNP Q5UPL1
Ι	-1	GLY	-	expression tag	UNP Q5UPL1
Ι	0	HIS	-	expression tag	UNP Q5UPL1
J	-3	GLY	-	expression tag	UNP Q5UPL1
J	-2	GLY	-	expression tag	UNP Q5UPL1
J	-1	GLY	-	expression tag	UNP Q5UPL1
J	0	HIS	-	expression tag	UNP Q5UPL1

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• Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: $C_8H_{13}N_2O_5P$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
9	Δ	1	Total	С	Ν	0	Р	0	0
	A	1	16	8	2	5	1	0	0
2	В	1	Total	С	Ν	Ο	Р	0	0
	D	1	16	8	2	5	1	0	0
2	С	1	Total	С	Ν	Ο	Р	0	0
	U	1	16	8	2	5	1	0	0
2	Л	1	Total	С	Ν	Ο	Р	0	0
2	D	T	16	8	2	5	1	0	0
2	E	1	Total	С	Ν	Ο	Р	0	0
2	Ľ	1	16	8	2	5	1	0	0
2	F	1	Total	С	Ν	Ο	Р	0	0
	T	1	16	8	2	5	1	0	0
2	G	1	Total	С	Ν	Ο	Р	0	0
2	ŭ	1	16	8	2	5	1	0	0
2	н	1	Total	С	Ν	Ο	Р	0	0
2	11	1	16	8	2	5	1	0	0
2	T	1	Total	С	N	Ō	Р	0	0
	L	1	16	8	2	5	1	0	U
2	т	1	Total	С	Ν	0	Р	0	0
	1		16	8	2	5	1		U

• Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	А	1	Total 5	0 4	Р 1	0	0

• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	J	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	J	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total Cl 1 1	0	0

• Molecule 6 is THYMIDINE-5'-DIPHOSPHATE (three-letter code: TYD) (formula: $C_{10}H_{16}N_2O_{11}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
6	р	1	Total	С	Ν	Ο	Р	0	0	
0 D	L	25	10	2	11	2	0	0		
6	6 B	B 1	Total	С	Ν	Ο	Р	0	0	
0			25	10	2	11	2	0		
6	C	1	Total	С	Ν	Ο	Р	0	0	
0	U		25	10	2	11	2	0	0	



Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf			
6	Л	1	Total	С	Ν	Ο	Р	0	0			
0	D	1	25	10	2	11	2	0	0			
6	6 E	F	Ţ	s F	1	Total	С	Ν	Ο	Р	0	0
0		1	25	10	2	11	2	0	0			
6	F	1	Total	С	Ν	Ο	Р	0	0			
0 E	I	25	10	2	11	2	0	0				
6		G 1	Total	С	Ν	Ο	Р	0	0			
0	G		25	10	2	11	2					
6	Ц	1	Total	С	Ν	Ο	Р	0	0			
0	11	I	25	10	2	11	2	0	0			
6	т	1	Total	С	Ν	Ο	Р	0	0			
0 1	1	25	10	2	11	2	0	0				
6	T	T 1	Total	С	Ν	0	Р	0	0			
0 J	1	25	10	2	11	2	0	U				

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• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	362	Total O 362 362	0	0
7	В	331	Total O 331 331	0	0
7	С	332	Total O 332 332	0	0
7	D	232	Total O 232 232	0	0
7	Е	380	Total O 380 380	0	0
7	F	344	Total O 344 344	0	0
7	G	226	Total O 226 226	0	0
7	Н	264	Total O 264 264	0	0
7	Ι	167	Total O 167 167	0	0
7	J	276	Total O 276 276	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: L136 aminotransferase







• Molecule 1: L136 aminotransferase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	74.89Å 126.88Å 206.37Å	Deperitor
a, b, c, α , β , γ	90.00° 90.89° 90.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	33.78 - 1.70	Depositor
Resolution (A)	33.76 - 1.70	EDS
% Data completeness	94.2 (33.78-1.70)	Depositor
(in resolution range)	94.3 (33.76-1.70)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	0.06	Depositor
$< I/\sigma(I) > 1$	5.77 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
D D.	0.182 , 0.222	Depositor
Π, Π_{free}	0.192 , 0.230	DCC
R_{free} test set	19828 reflections $(4.99%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	19.7	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.42, 51.3	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	31417	wwPDB-VP
Average B, all atoms $(Å^2)$	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PO4, EDO, PMP, TYD

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	Bo	nd lengths	Bond angles		
1VIOI	Ullaill	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.77	1/2844~(0.0%)	0.86	0/3848	
1	В	0.75	0/2878	0.86	0/3895	
1	С	0.73	0/2878	0.84	0/3896	
1	D	0.76	0/2873	0.85	0/3887	
1	Е	0.74	0/2896	0.86	0/3916	
1	F	0.78	0/2865	0.88	1/3877~(0.0%)	
1	G	0.76	1/2870~(0.0%)	0.84	1/3882~(0.0%)	
1	Н	0.74	0/2865	0.82	0/3877	
1	Ι	0.75	0/2853	0.87	0/3861	
1	J	0.73	0/2873	0.84	0/3886	
All	All	0.75	2/28695~(0.0%)	0.85	2/38825~(0.0%)	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
1	G	66	SER	CA-CB	-6.00	1.44	1.52
1	А	257	GLU	CD-OE1	5.51	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	F	77	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	G	323	ARG	NE-CZ-NH2	-5.26	117.67	120.30

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	2783	0	2752	15	1
1	В	2810	0	2785	20	0
1	С	2811	0	2779	13	0
1	D	2808	0	2777	23	0
1	Е	2831	0	2813	27	0
1	F	2801	0	2771	23	0
1	G	2809	0	2784	22	0
1	Н	2801	0	2775	14	0
1	Ι	2792	0	2761	37	1
1	J	2809	0	2790	24	0
2	А	16	0	10	0	0
2	В	16	0	10	0	0
2	С	16	0	10	0	0
2	D	16	0	10	0	0
2	Е	16	0	11	0	0
2	F	16	0	11	0	0
2	G	16	0	10	0	0
2	Н	16	0	11	0	0
2	Ι	16	0	11	0	0
2	J	16	0	10	0	0
3	А	5	0	0	0	0
4	А	4	0	6	0	0
4	В	8	0	12	0	0
4	С	4	0	6	0	0
4	Е	4	0	6	1	0
4	F	4	0	6	0	0
4	J	8	0	12	0	0
5	А	1	0	0	0	0
6	В	50	0	26	11	0
6	С	25	0	13	3	0
6	D	25	0	13	0	0
6	Е	50	0	26	20	0
6	G	25	0	13	0	0
6	Н	25	0	13	0	0
6	Ι	25	0	13	2	0
6	J	25	0	13	1	0
7	А	362	0	0	1	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	В	331	0	0	4	0
7	С	332	0	0	3	0
7	D	232	0	0	0	0
7	Е	380	0	0	7	0
7	F	344	0	0	2	0
7	G	226	0	0	5	0
7	Н	264	0	0	1	0
7	Ι	167	0	0	2	0
7	J	276	0	0	7	0
All	All	31417	0	28069	211	1

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The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 211 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)
6:B:403:TYD:O2B	7:B:501:HOH:O	1.89	0.90
6:C:402:TYD:H5'2	1:D:304:ARG:HH12	1.37	0.88
1:E:304:ARG:HH22	6:E:402:TYD:C3'	1.86	0.88
1:G:168:LYS:HE3	7:G:506:HOH:O	1.74	0.88
6:B:403:TYD:O3B	7:B:502:HOH:O	1.99	0.80

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ASP:OD2	1:I:295:ARG:NH2[2_647]	2.08	0.12

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	346/356~(97%)	335~(97%)	10 (3%)	1 (0%)	41	24
1	В	350/356~(98%)	339~(97%)	10 (3%)	1 (0%)	41	24
1	С	352/356~(99%)	338~(96%)	13 (4%)	1 (0%)	41	24
1	D	350/356~(98%)	338~(97%)	11 (3%)	1 (0%)	41	24
1	Е	352/356~(99%)	341 (97%)	10 (3%)	1 (0%)	41	24
1	F	349/356~(98%)	336 (96%)	12 (3%)	1 (0%)	41	24
1	G	350/356~(98%)	333~(95%)	16 (5%)	1 (0%)	41	24
1	Н	350/356~(98%)	338~(97%)	11 (3%)	1 (0%)	41	24
1	Ι	348/356~(98%)	333 (96%)	14 (4%)	1 (0%)	41	24
1	J	350/356~(98%)	342 (98%)	7 (2%)	1 (0%)	41	24
All	All	3497/3560~(98%)	3373 (96%)	114 (3%)	10 (0%)	41	24

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	Е	35	ILE
1	D	35	ILE
1	Н	35	ILE
1	J	35	ILE
1	В	35	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	312/317~(98%)	305~(98%)	7~(2%)	52 34
1	В	315/317~(99%)	309~(98%)	6 (2%)	57 41
1	С	314/317~(99%)	309~(98%)	5(2%)	62 48
1	D	314/317~(99%)	312~(99%)	2(1%)	86 80
1	Ε	318/317~(100%)	313~(98%)	5(2%)	62 48
1	F	314/317~(99%)	312 (99%)	2 (1%)	86 80



Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	G	314/317~(99%)	307~(98%)	7(2%)	52 34		
1	Н	313/317~(99%)	305~(97%)	8 (3%)	46 28		
1	Ι	312/317~(98%)	305~(98%)	7 (2%)	52 34		
1	J	315/317~(99%)	306~(97%)	9~(3%)	42 23		
All	All	3141/3170~(99%)	3083~(98%)	58 (2%)	57 43		

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5 of 58 residues with a non-rotameric side chain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	G	147	MET
1	J	302	LEU
1	Н	77	ARG
1	J	295	ARG
1	J	77	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	Н	236	ASN
1	J	236	ASN
1	Ι	96	ASN
1	Ι	352	ASN
1	D	236	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 30 ligands modelled in this entry, 1 is monoatomic - leaving 29 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Bos	Link	Bo	ond leng	ths	B	Bond angles		
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
2	PMP	В	402	-	16,16,16	0.76	0	21,23,23	0.93	1 (4%)	
4	EDO	F	402	-	3,3,3	0.41	0	2,2,2	0.31	0	
3	PO4	А	402	-	4,4,4	1.13	1 (25%)	6,6,6	0.47	0	
2	PMP	Е	401	-	16,16,16	0.57	0	21,23,23	1.12	2 (9%)	
4	EDO	J	404	-	3,3,3	0.35	0	2,2,2	0.20	0	
6	TYD	В	403	-	23,26,26	1.91	3 (13%)	33,40,40	1.72	4 (12%)	
4	EDO	В	404	-	3,3,3	0.45	0	2,2,2	0.34	0	
6	TYD	J	401	-	23,26,26	1.88	3 (13%)	33,40,40	1.60	3 (9%)	
6	TYD	Н	401	-	23,26,26	1.93	3 (13%)	33,40,40	1.64	3 (9%)	
2	PMP	А	401	-	16,16,16	0.52	0	21,23,23	0.79	0	
2	PMP	Ι	401	-	16,16,16	0.49	0	21,23,23	0.80	1 (4%)	
2	PMP	D	402	-	16,16,16	0.67	0	21,23,23	1.03	1 (4%)	
4	EDO	J	403	-	3,3,3	0.81	0	2,2,2	0.65	0	
6	TYD	Ι	402	-	23,26,26	1.84	2 (8%)	33,40,40	1.67	5 (15%)	
6	TYD	В	401	-	23,26,26	1.89	6 (26%)	33,40,40	1.86	4 (12%)	
6	TYD	С	402	-	23,26,26	1.85	2 (8%)	33,40,40	1.78	5 (15%)	
2	PMP	С	401	-	16,16,16	0.55	0	21,23,23	0.85	0	
2	PMP	G	401	-	16,16,16	0.48	0	21,23,23	1.13	1 (4%)	
6	TYD	G	402	-	23,26,26	1.88	4 (17%)	33,40,40	1.67	3 (9%)	
4	EDO	В	405	-	3,3,3	0.32	0	2,2,2	0.17	0	
6	TYD	Е	402	-	23,26,26	1.78	2 (8%)	33,40,40	1.76	5(15%)	
2	PMP	J	402	-	16,16,16	0.77	0	21,23,23	1.02	2 (9%)	
6	TYD	D	401	-	23,26,26	1.83	3 (13%)	33,40,40	1.75	6 (18%)	
4	EDO	А	403	-	3,3,3	0.28	0	2,2,2	0.23	0	
2	PMP	Н	402	-	16,16,16	1.89	3 (18%)	21,23,23	1.49	6 (28%)	
4	EDO	С	403	-	3,3,3	0.18	0	2,2,2	0.11	0	
6	TYD	Е	403	-	23,26,26	1.89	2 (8%)	33,40,40	1.73	5 (15%)	
4	EDO	Е	404	-	3,3,3	0.15	0	2,2,2	0.62	0	



Mol Typ	Tuno	Chain	Chain	Dog	Tink	Bo	ond leng	ths	B	ond ang	les
	туре		nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	PMP	F	401	-	16,16,16	0.56	0	21,23,23	0.91	1 (4%)	

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	PMP	В	402	-	-	1/8/8/8	0/1/1/1
4	EDO	F	402	-	-	0/1/1/1	-
2	PMP	Е	401	-	-	2/8/8/8	0/1/1/1
4	EDO	J	404	-	-	0/1/1/1	-
6	TYD	В	403	-	-	1/16/28/28	0/2/2/2
4	EDO	В	404	-	-	1/1/1/1	-
6	TYD	J	401	-	-	0/16/28/28	0/2/2/2
6	TYD	Н	401	-	-	1/16/28/28	0/2/2/2
2	PMP	А	401	-	-	2/8/8/8	0/1/1/1
2	PMP	Ι	401	-	-	2/8/8/8	0/1/1/1
2	PMP	D	402	-	-	0/8/8/8	0/1/1/1
4	EDO	J	403	-	-	1/1/1/1	-
6	TYD	Ι	402	-	-	0/16/28/28	0/2/2/2
6	TYD	В	401	-	-	0/16/28/28	0/2/2/2
6	TYD	С	402	-	-	1/16/28/28	0/2/2/2
2	PMP	С	401	-	-	2/8/8/8	0/1/1/1
2	PMP	G	401	-	-	2/8/8/8	0/1/1/1
6	TYD	G	402	-	-	1/16/28/28	0/2/2/2
4	EDO	В	405	-	-	0/1/1/1	-
6	TYD	Е	402	-	-	1/16/28/28	0/2/2/2
2	PMP	J	402	-	-	0/8/8/8	0/1/1/1
6	TYD	D	401	-	-	0/16/28/28	0/2/2/2
4	EDO	А	403	-	-	0/1/1/1	-
2	PMP	Н	402	-	-	2/8/8/8	0/1/1/1
4	EDO	С	403	-	-	0/1/1/1	-
6	TYD	Е	403	-	-	1/16/28/28	0/2/2/2
4	EDO	Е	404	-	-	0/1/1/1	-
2	PMP	F	401	_	_	2/8/8/8	0/1/1/1

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
6	Е	403	TYD	C6-N1	-6.58	1.38	1.46



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	В	403	TYD	C6-N1	-6.38	1.38	1.46
6	С	402	TYD	C6-N1	-6.28	1.38	1.46
6	Н	401	TYD	C6-N1	-6.25	1.38	1.46
6	J	401	TYD	C6-N1	-6.25	1.38	1.46

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The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	В	401	TYD	C5-C6-N1	6.66	124.23	111.11
6	J	401	TYD	C5-C6-N1	6.50	123.92	111.11
6	G	402	TYD	C5-C6-N1	6.40	123.72	111.11
6	Н	401	TYD	C5-C6-N1	6.37	123.65	111.11
6	Е	403	TYD	C5-C6-N1	6.34	123.61	111.11

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	401	PMP	C3-C4-C4A-N4A
2	А	401	PMP	C5-C4-C4A-N4A
2	С	401	PMP	C5-C4-C4A-N4A
2	G	401	PMP	C3-C4-C4A-N4A
2	G	401	PMP	C5-C4-C4A-N4A

There are no ring outliers.

8 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	В	403	TYD	10	0
6	J	401	TYD	1	0
6	Ι	402	TYD	2	0
6	В	401	TYD	1	0
6	С	402	TYD	3	0
6	Е	402	TYD	10	0
6	Е	403	TYD	10	0
4	Е	404	EDO	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	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	348/356~(97%)	-0.04	8 (2%) 60 65	12, 19, 33, 53	0
1	В	350/356~(98%)	0.11	8 (2%) 60 65	11, 20, 39, 58	0
1	С	352/356~(98%)	-0.04	9 (2%) 56 60	13, 19, 38, 57	0
1	D	351/356~(98%)	0.30	16 (4%) 32 36	13, 27, 45, 81	0
1	Ε	353/356~(99%)	-0.01	7 (1%) 65 69	11, 20, 37, 50	0
1	F	350/356~(98%)	0.04	9 (2%) 56 60	12, 20, 37, 68	0
1	G	352/356~(98%)	0.48	16 (4%) 33 37	19, 28, 43, 76	0
1	Η	351/356~(98%)	0.30	14 (3%) 38 42	16, 25, 44, 63	0
1	Ι	350/356~(98%)	0.87	38 (10%) 5 6	18, 32, 50, 63	0
1	J	351/356~(98%)	0.22	9 (2%) 56 60	14, 24, 43, 66	0
All	All	3508/3560~(98%)	0.22	134 (3%) 40 45	11, 23, 42, 81	0

The worst 5 of 134 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Н	2	GLY	5.8
1	В	312	LEU	5.3
1	D	312	LEU	4.7
1	D	120	LYS	4.4
1	D	2	GLY	4.3

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
4	EDO	J	403	4/4	0.66	0.22	34,39,39,39	0
6	TYD	G	402	25/25	0.73	0.24	35,53,74,81	0
4	EDO	В	404	4/4	0.84	0.13	29,30,31,35	0
6	TYD	Ι	402	25/25	0.84	0.20	36,49,66,74	0
6	TYD	J	401	25/25	0.84	0.19	30,45,69,76	0
6	TYD	С	402	25/25	0.85	0.21	27,44,64,79	0
6	TYD	В	403	25/25	0.85	0.22	25,43,77,84	0
6	TYD	Н	401	25/25	0.87	0.17	28,38,60,70	0
6	TYD	Е	403	25/25	0.88	0.16	21,34,71,79	0
6	TYD	Е	402	25/25	0.90	0.14	19,33,68,79	0
3	PO4	А	402	5/5	0.92	0.21	44,44,53,55	0
6	TYD	D	401	25/25	0.92	0.11	21,28,67,73	0
6	TYD	В	401	25/25	0.92	0.11	17,26,57,67	0
4	EDO	F	402	4/4	0.92	0.12	26,31,32,35	0
4	EDO	J	404	4/4	0.93	0.10	22,25,26,28	0
4	EDO	С	403	4/4	0.94	0.14	25,29,30,30	0
4	EDO	Е	404	4/4	0.95	0.14	31,36,40,44	0
4	EDO	А	403	4/4	0.95	0.10	27,28,29,30	0
2	PMP	G	401	16/16	0.96	0.14	19,22,28,36	0
2	PMP	Н	402	16/16	0.96	0.11	19,21,28,34	0
2	PMP	Ι	401	16/16	0.97	0.16	20,26,34,43	0
5	CL	А	404	1/1	0.97	0.06	26,26,26,26	0
4	EDO	В	405	4/4	0.97	0.07	24,25,28,29	0
2	PMP	J	402	16/16	0.97	0.12	15,19,25,31	0
2	PMP	А	401	16/16	0.98	0.15	11,14,20,26	0
2	PMP	В	402	16/16	0.98	0.12	12,13,19,27	0
2	PMP	С	401	16/16	0.98	0.16	12,14,19,25	0
2	PMP	D	402	16/16	0.98	0.10	15,21,24,33	0
2	PMP	Е	401	16/16	0.98	0.16	11,14,19,26	0
2	PMP	F	401	16/16	0.98	0.14	11,15,22,30	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.

