

# wwPDB X-ray Structure Validation Summary Report (i)

#### Feb 22, 2021 – 11:15 AM GMT

PDB ID	:	6ZG3
$\operatorname{Title}$	:	the structure of ECF PanT transporter in a complex with a nanobody
Authors	:	Setyawati, I.; Guskov, A.; Slotboom, D.J.
Deposited on	:	2020-06-18
Resolution	:	2.80  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 09b 467
Mon robity	•	4.020-407
Mogul	:	$1.8.5 \ (274361), \ \text{CSD} \ \text{as}541 \text{be} \ (2020)$
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.17.1.dev1
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{Refmac}$	:	5.8.0158
$\operatorname{CCP4}$	:	7.0.044  (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	$2.17.1.  m{dev1}$

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution $(#Entries, resolution range(Å))$		
D				
$\mathbf{R}_{free}$	130704	3140(2.80-2.80)		
Clashscore	141614	3569(2.80-2.80)		
Ramachandran outliers	138981	3498 (2.80-2.80)		
Sidechain outliers	138945	3500 (2.80-2.80)		
RSRZ outliers	127900	3078 (2.80-2.80)		

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 chair	1	
-		200	2%		
	A	300	56%	33%	5% 7%
			4%		
1	F	300	62%	28%	• 7%
			13%		
2	В	287	64%	32%	••
			9%		
2	G	287	59%	37%	• •
			6%		
3	С	215	61%	32%	• •



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Mol	Chain	Length	Quality of cha	ain	
3	Н	215	60%	32%	5% •
4	D	265	58%	34%	5% •
4	Ι	265	62%	32%	5% •
5	Е	136	48%	40%	• 7%
5	J	136	4% 54%	37%	• 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	PEG	D	303	-	-	-	Х
7	LMT	С	502	-	-	-	Х
7	LMT	D	301	-	-	-	Х



# 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 18233 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	280	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
	А	280	2147	1354	359	430	4	0	0	0
1	Б	270	Total	С	Ν	Ο	S	0	0	0
	Г	219	2143	1352	358	429	4	0	0	0

• Molecule 1 is a protein called Energy-coupling factor transporter ATP-binding protein EcfA1.

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP Q1GBJ0
A	-16	HIS	-	expression tag	UNP Q1GBJ0
A	-15	HIS	-	expression tag	UNP Q1GBJ0
A	-14	HIS	-	expression tag	UNP Q1GBJ0
A	-13	HIS	-	expression tag	UNP Q1GBJ0
A	-12	HIS	-	expression tag	UNP Q1GBJ0
A	-11	HIS	-	expression tag	UNP Q1GBJ0
A	-10	HIS	-	expression tag	UNP Q1GBJ0
A	-9	HIS	-	expression tag	UNP Q1GBJ0
A	-8	HIS	-	expression tag	UNP Q1GBJ0
A	-7	HIS	-	expression tag	UNP Q1GBJ0
A	-6	GLY	-	expression tag	UNP Q1GBJ0
A	-5	GLU	-	expression tag	UNP Q1GBJ0
A	-4	ASN	-	expression tag	UNP Q1GBJ0
A	-3	LEU	-	expression tag	UNP Q1GBJ0
A	-2	TYR	-	expression tag	UNP Q1GBJ0
A	-1	PHE	-	expression tag	UNP Q1GBJ0
A	0	GLN	-	expression tag	UNP Q1GBJ0
A	1	GLY	-	expression tag	UNP Q1GBJ0
F	-17	MET	-	initiating methionine	UNP Q1GBJ0
F	-16	HIS	-	expression tag	UNP Q1GBJ0
F	-15	HIS	-	expression tag	UNP Q1GBJ0
F	-14	HIS	-	expression tag	UNP Q1GBJ0
F	-13	HIS	-	expression tag	UNP Q1GBJ0
F	-12	HIS	-	expression tag	UNP Q1GBJ0

There are 38 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	$\mathbf{Comment}$	Reference
F	-11	HIS	-	expression tag	UNP Q1GBJ0
F	-10	HIS	-	expression tag	UNP Q1GBJ0
F	-9	HIS	-	expression tag	UNP Q1GBJ0
F	-8	HIS	-	expression tag	UNP Q1GBJ0
F	-7	HIS	-	expression tag	UNP Q1GBJ0
F	-6	GLY	-	expression tag	UNP Q1GBJ0
F	-5	GLU	-	expression tag	UNP Q1GBJ0
F	-4	ASN	-	expression tag	UNP Q1GBJ0
F	-3	LEU	-	expression tag	UNP Q1GBJ0
F	-2	TYR	-	expression tag	UNP Q1GBJ0
F	-1	PHE	-	expression tag	UNP Q1GBJ0
F	0	GLN	-	expression tag	UNP Q1GBJ0
F	1	GLY	-	expression tag	UNP Q1GBJ0

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• Molecule 2 is a protein called Energy-coupling factor transporter ATP-binding protein EcfA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	В	282	Total	С	Ν	Ο	S	0	0	0
	D		2187	1396	371	412	8	0		
0	C	002	Total	С	Ν	0	S	0	0	0
	G	200	2195	1401	372	413	9	0	0	0

• Molecule 3 is a protein called Conserved hypothetical membrane protein.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	C	20.7	Total	С	Ν	Ο	S	0	0	0
0		201	1553	1033	257	262	1	0		
2	и	20.7	Total	С	Ν	Ο	S	0	0	0
J	11	207	1553	1033	257	262	1	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	208	TRP	-	expression tag	UNP Q1GBG0
С	209	SER	-	expression tag	UNP Q1GBG0
С	210	HIS	-	expression tag	UNP Q1GBG0
С	211	PRO	-	expression tag	UNP Q1GBG0
С	212	GLN	-	expression tag	UNP Q1GBG0
С	213	PHE	-	expression tag	UNP Q1GBG0
С	214	GLU	-	expression tag	UNP Q1GBG0
С	215	LYS	-	expression tag	UNP Q1GBG0
Н	208	TRP	-	expression tag	UNP Q1GBG0



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Chain	Residue	Modelled	Actual	Comment	Reference					
Η	209	SER	-	expression tag	UNP Q1GBG0					
Η	210	HIS	-	expression tag	UNP Q1GBG0					
Η	211	PRO	-	expression tag	UNP Q1GBG0					
Н	212	GLN	-	expression tag	UNP Q1GBG0					
Н	213	PHE	-	expression tag	UNP Q1GBG0					
Н	214	GLU	-	expression tag	UNP Q1GBG0					
Н	215	LYS	-	expression tag	UNP Q1GBG0					

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• Molecule 4 is a protein called Putative cobalt ABC transporter, permease protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	а	260	Total	С	Ν	Ο	S	0	1	0
4	4 D	200	2105	1406	337	348	14	0	L	0
4	т	260	Total	С	Ν	Ο	S	0	0	0
4	4 1	200	2093	1397	336	346	14			

• Molecule 5 is a protein called CA14381 nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	5 E	126	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
0			964	603	164	192	5	0		
5	т	195	Total	С	Ν	0	S	0	0	0
9 J	120	955	598	162	190	5	U	0	U	

• Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).





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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
6	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
6	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
6	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
6	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
6	D	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
6	D	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
6	Е	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
6	Ι	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
6	J	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0

• Molecule 7 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



		iteslates	Atoms			LeroOcc	AltConf
7	С	1	Total 32	C 21	0 11	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	С	1	Total C O 35 24 11	0	0
7	D	1	Total         C         O           35         24         11	0	0
7	G	1	Total         C         O           35         24         11	0	0
7	Н	1	Total         C         O           35         24         11	0	0
7	Н	1	Total         C         O           35         24         11	0	0
7	Ι	1	Total         C         O           35         24         11	0	0

• Molecule 8 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	С	1	Total         C         O           13         6         7	0	0
8	Н	1	Total         C         O           13         6         7	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: Energy-coupling factor transporter ATP-binding protein EcfA1



• Molecule 1: Energy-coupling factor transporter ATP-binding protein EcfA1



• Molecule 2: Energy-coupling factor transporter ATP-binding protein EcfA2

Chain B:

13%













#### L204 K205 R206 R207 TRP SER H1S PR0 GLN GLN CLU

• Molecule 4: Putative cobalt ABC transporter, permease protein



• Molecule 4: Putative cobalt ABC transporter, permease protein





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• Molecule 5: CA14381 nanobody







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	97.29Å $110.47$ Å $110.50$ Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$89.00^{\circ}$ $102.27^{\circ}$ $102.24^{\circ}$	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	48.83 - 2.80	Depositor
Resolution (A)	48.83 - 2.80	EDS
% Data completeness	96.4 (48.83-2.80)	Depositor
(in resolution range)	96.3(48.83-2.80)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.01 (at 2.81 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
D D	0.242 , $0.276$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.244 , $0.276$	DCC
$R_{free}$ test set	5214 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	85.1	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.27, $54.2$	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.49, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.378 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	18233	wwPDB-VP
Average B, all atoms $(Å^2)$	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: CIT, LMT, PEG

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	Bo	ond angles
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.50	0/2180	0.73	1/2959~(0.0%)
1	F	0.50	0/2176	0.70	0/2954
2	В	0.42	0/2233	0.65	0/3014
2	G	0.42	0/2241	0.65	0/3024
3	С	0.46	0/1584	0.73	0/2164
3	Н	0.45	0/1584	0.71	0/2164
4	D	0.50	0/2160	0.68	1/2934~(0.0%)
4	Ι	0.49	0/2147	0.69	2/2916~(0.1%)
5	Е	0.59	1/987~(0.1%)	0.75	1/1342~(0.1%)
5	J	0.59	1/978~(0.1%)	0.73	0/1330
All	All	0.48	2/18270~(0.0%)	0.70	5/24801~(0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
5	J	50	CYS	CB-SG	-6.92	1.70	1.82
5	Е	106	CYS	CB-SG	-6.11	1.71	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
4	D	81	LEU	CA-CB-CG	8.09	133.90	115.30
5	Е	106	CYS	CA-CB-SG	-6.20	102.85	114.00
1	А	222	LEU	CA-CB-CG	-5.41	102.86	115.30
4	Ι	193	LEU	CB-CG-CD1	-5.30	101.99	111.00
4	Ι	193	LEU	CA-CB-CG	5.30	127.48	115.30

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	2147	0	2159	80	0
1	F	2143	0	2153	71	0
2	В	2187	0	2190	70	0
2	G	2195	0	2202	98	0
3	С	1553	0	1697	64	0
3	Н	1553	0	1697	73	0
4	D	2105	0	2200	69	0
4	Ι	2093	0	2192	69	0
5	Е	964	0	913	48	0
5	J	955	0	902	31	0
6	А	7	0	10	1	0
6	В	7	0	10	0	0
6	С	21	0	30	2	0
6	D	14	0	20	0	0
6	Е	7	0	10	0	0
6	Ι	7	0	10	0	0
6	J	7	0	10	1	0
7	С	67	0	83	4	0
7	D	35	0	46	4	0
7	G	35	0	46	5	0
7	Н	70	0	92	7	0
7	Ι	35	0	46	2	0
8	С	13	0	5	1	0
8	Н	13	0	5	1	0
All	All	18233	0	18728	630	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 17.

The worst 5 of 630 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:F:12:THR:HG22	1:F:25:ASP:H	1.20	1.03
2:G:6:GLU:O	2:G:62:GLY:HA3	1.68	0.94
1:A:12:THR:HG22	1:A:25:ASP:H	1.35	0.90



Atom 1	Atom D	Interatomic	Clash							
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)							
2:G:248:ARG:HH11	2:G:251:ARG:HH11	1.18	0.88							
5:J:67:ARG:NH2	5:J:90:ASP:OD2	2.08	0.87							

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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	entiles
1	А	278/300~(93%)	264~(95%)	12 (4%)	2(1%)	22	53
1	F	277/300~(92%)	264 (95%)	12 (4%)	1 (0%)	34	66
2	В	280/287~(98%)	269~(96%)	10 (4%)	1 (0%)	34	66
2	G	281/287~(98%)	274 (98%)	7 (2%)	0	100	100
3	С	205/215~(95%)	198 (97%)	6 (3%)	1 (0%)	29	61
3	Н	205/215~(95%)	199 (97%)	6 (3%)	0	100	100
4	D	259/265~(98%)	245~(95%)	11 (4%)	3 (1%)	13	39
4	Ι	258/265~(97%)	242 (94%)	15 (6%)	1 (0%)	34	66
5	Е	124/136~(91%)	118 (95%)	5 (4%)	1 (1%)	19	49
5	J	123/136~(90%)	119 (97%)	4 (3%)	0	100	100
All	All	2290/2406~(95%)	2192 (96%)	88 (4%)	10 (0%)	34	66

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	44	SER
5	Е	3	GLN
1	F	44	SER
2	В	260	GLY
4	D	8	ARG



#### 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	entiles
1	А	240/259~(93%)	223~(93%)	17 (7%)	14	39
1	F	240/259~(93%)	223~(93%)	17 (7%)	14	39
2	В	230/234~(98%)	220~(96%)	10 (4%)	29	62
2	G	231/234~(99%)	219~(95%)	12 (5%)	23	55
3	С	162/170~(95%)	149~(92%)	13 (8%)	12	34
3	Н	162/170~(95%)	147 (91%)	15~(9%)	9	26
4	D	229/233~(98%)	196~(86%)	33 (14%)	3	10
4	Ι	228/233~(98%)	199~(87%)	29 (13%)	4	14
5	Ε	103/112~(92%)	94 (91%)	9 (9%)	10	30
5	J	102/112~(91%)	96 (94%)	6 (6%)	19	49
All	All	1927/2016~(96%)	1766 (92%)	161 (8%)	11	31

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Н	77	ARG
4	Ι	129	THR
3	Н	136	SER
4	Ι	40	ASN
4	Ι	220	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	40	ASN
1	F	41	HIS

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

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

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

19 ligands are modelled in this entry.

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

Mal	Tuno	Chain	Dog	Bes Link Bond lengths Bond a				ond ang	gles	
MOI	туре	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
7	LMT	Η	601	-	36, 36, 36	1.07	1 (2%)	$47,\!47,\!47$	1.24	8 (17%)
6	PEG	Е	201	-	$6,\!6,\!6$	0.49	0	5, 5, 5	0.40	0
6	PEG	С	505	-	$6,\!6,\!6$	0.50	0	5, 5, 5	0.26	0
8	CIT	С	503	-	$3,\!12,\!12$	1.40	1(33%)	$3,\!17,\!17$	1.64	<mark>1 (33%)</mark>
7	LMT	С	502	-	36, 36, 36	1.09	4 (11%)	$47,\!47,\!47$	1.09	3 (6%)
7	LMT	С	501	-	$33,\!33,\!36$	1.11	2(6%)	44,44,47	1.10	4 (9%)
7	LMT	D	301	-	36, 36, 36	1.14	3 (8%)	47,47,47	1.15	5(10%)
6	PEG	В	301	-	$6,\!6,\!6$	0.51	0	5, 5, 5	0.38	0
8	CIT	Н	602	-	$3,\!12,\!12$	1.51	1(33%)	$3,\!17,\!17$	0.39	0
7	LMT	Η	603	-	36, 36, 36	1.05	3 (8%)	$47,\!47,\!47$	1.86	13 (27%)
7	LMT	Ι	301	-	36, 36, 36	1.10	2 (5%)	47,47,47	1.59	10 (21%)
6	PEG	D	303	-	$6,\!6,\!6$	0.64	0	5, 5, 5	0.67	0
6	PEG	А	301	-	$6,\!6,\!6$	0.57	0	5, 5, 5	0.40	0
7	LMT	G	901	-	$36, \! 36, \! 36$	1.09	4 (11%)	$47,\!47,\!47$	1.29	<mark>6 (12%)</mark>
6	PEG	С	506	-	$6,\!6,\!6$	0.51	0	5, 5, 5	0.38	0
6	PEG	D	302	-	$6,\!6,\!6$	0.50	0	5, 5, 5	0.29	0
6	PEG	Ι	302	-	6,6,6	0.49	0	5, 5, 5	0.35	0
6	PEG	С	504	-	6,6,6	0.51	0	5, 5, 5	0.24	0
6	PEG	J	201	-	6,6,6	0.50	0	5, 5, 5	0.52	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
7	LMT	Н	601	-	-	14/21/61/61	0/2/2/2
6	PEG	Е	201	-	-	0/4/4/4	-
6	PEG	C	505	-	-	2/4/4/4	-
8	CIT	С	503	-	-	6/6/16/16	-
7	LMT	С	502	-	-	11/21/61/61	0/2/2/2
7	LMT	С	501	-	-	8/18/58/61	0/2/2/2
7	LMT	D	301	-	-	11/21/61/61	0/2/2/2
6	PEG	В	301	-	-	3/4/4/4	-
8	CIT	Н	602	-	-	3/6/16/16	-
7	LMT	Н	603	-	-	9/21/61/61	0/2/2/2
7	LMT	Ι	301	-	-	16/21/61/61	0/2/2/2
6	PEG	D	303	-	-	2/4/4/4	-
6	PEG	А	301	-	-	1/4/4/4	-
7	LMT	G	901	-	-	14/21/61/61	0/2/2/2
6	PEG	С	506	-	-	1/4/4/4	-
6	PEG	D	302	-	-	2/4/4/4	-
6	PEG	Ι	302	-	-	3/4/4/4	-
6	PEG	С	504	-	-	3/4/4/4	-
6	PEG	J	201	-	-	2/4/4/4	-

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
7	Ι	301	LMT	C4'-C5'	2.77	1.60	1.52
7	С	501	LMT	O3'-C3'	-2.52	1.37	1.43
7	Н	603	LMT	O3'-C3'	-2.51	1.37	1.43
7	D	301	LMT	O3'-C3'	-2.47	1.37	1.43
8	Н	602	CIT	O7-C3	2.43	1.46	1.43

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
7	Н	603	LMT	O5B-C5B-C4B	5.60	119.86	109.69
7	Н	603	LMT	C3'-C4'-C5'	-5.22	98.95	110.93
7	Ι	301	LMT	O1'-C1'-C2'	4.09	114.69	108.30



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	Ideal(°			
7	G	901	LMT	O1'-C1'-C2'	3.75	114.15	108.30			
7	Ι	301	LMT	O5'-C5'-C4'	3.73	117.61	109.75			

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There are no chirality outliers.

5 of 111 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	С	501	LMT	O5'-C1'-O1'-C1
7	D	301	LMT	C2-C1-O1'-C1'
7	G	901	LMT	C2'-C1'-O1'-C1
7	G	901	LMT	O5'-C1'-O1'-C1
7	G	901	LMT	C2-C1-O1'-C1'

There are no ring outliers.

12 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	Н	601	LMT	3	0
8	С	503	CIT	1	0
7	С	502	LMT	2	0
7	С	501	LMT	2	0
7	D	301	LMT	4	0
8	Н	602	CIT	1	0
7	Н	603	LMT	4	0
7	Ι	301	LMT	2	0
6	А	301	PEG	1	0
7	G	901	LMT	5	0
6	С	504	PEG	2	0
6	J	201	PEG	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	280/300~(93%)	-0.06	7 (2%) 57 47	58, 88, 140, 209	0
1	F	279/300~(93%)	0.12	12 (4%) 35 25	61, 88, 137, 222	0
2	В	282/287~(98%)	0.47	36~(12%) 3 2	77, 117, 164, 217	0
2	G	283/287~(98%)	0.38	27 (9%) 8 4	82, 117, 163, 226	0
3	С	207/215~(96%)	0.09	12 (5%) 23 15	73, 96, 166, 260	0
3	Н	207/215~(96%)	0.35	16 (7%) 13 7	71, 102, 175, 227	0
4	D	260/265~(98%)	0.49	27 (10%) 6 3	70, 118, 198, 257	0
4	Ι	260/265~(98%)	0.68	37~(14%) 2 1	66, 112, 187, 234	0
5	E	126/136~(92%)	-0.11	3 (2%) 59 49	63, 87, 124, 156	0
5	J	125/136~(91%)	0.00	5 (4%) 38 28	65, 89, 120, 138	0
All	All	$\boxed{2309/2406~(95\%)}$	0.28	182 (7%) 12 7	58, 104, 168, 260	0

The worst 5 of 182 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	1	MET	20.3
3	Н	33	GLY	12.0
2	В	2	ALA	11.1
4	Ι	100	THR	9.8
4	Ι	102	SER	9.0

## 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	${f B} ext{-factors}({f A}^2)$	Q<0.9
7	LMT	С	502	35/35	0.64	0.43	$96,\!140,\!160,\!170$	0
6	PEG	А	301	7/7	0.72	0.21	$97,\!98,\!105,\!110$	0
7	LMT	D	301	35/35	0.72	0.45	$108,\!129,\!143,\!147$	0
7	LMT	G	901	35/35	0.73	0.26	$115,\!149,\!157,\!159$	0
7	LMT	Ι	301	35/35	0.74	0.36	$82,\!139,\!173,\!175$	0
6	PEG	D	303	7/7	0.77	0.67	$98,\!100,\!115,\!124$	0
7	LMT	Н	601	35/35	0.79	0.20	82,131,172,172	0
6	PEG	С	504	7/7	0.80	0.11	104,116,122,124	0
7	LMT	С	501	32/35	0.82	0.19	$81,\!136,\!165,\!168$	0
8	CIT	С	503	13/13	0.83	0.13	132,141,149,191	0
6	PEG	Ι	302	7/7	0.84	0.50	$88,\!103,\!110,\!111$	0
7	LMT	Н	603	35/35	0.84	0.26	$97,\!137,\!156,\!161$	0
6	PEG	С	506	7/7	0.85	0.32	101,106,117,122	0
8	CIT	Н	602	13/13	0.86	0.13	111,122,134,137	0
6	PEG	Е	201	7/7	0.88	0.17	71,82,92,93	0
6	PEG	В	301	7/7	0.90	0.41	102,114,119,121	0
6	PEG	С	505	7/7	0.91	0.11	114,116,125,127	0
6	PEG	D	302	7/7	0.92	0.10	$119,\!125,\!130,\!130$	0
6	PEG	J	201	7/7	0.95	0.23	72,79,82,84	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.

