

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

#### Nov 22, 2023 – 12:05 AM JST

:	8JIB
:	Crystal Structure of Prophenoloxidase PPO6 from Aedes aegypti
:	Zhu, X.; Zhang, L.; Yang, X.; Bao, P.; Ren, D.; Han, Q.
:	2023-05-26
:	3.15  Å(reported)
	::

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

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 3.15 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 <sub>free</sub>	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)

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%

Mol	Chain	Length	Quality of chain	
1	А	681	71% 20%	5% •
1	В	681	72% 19%	•• 5%
1	С	681	71% 20%	•• 5%
1	D	681	72% 20%	• 5%
1	Е	681	72% 219	6 • •
1	F	681	73% 18%	5 • •
1	G	681	77%	17% • •



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Mol	Chain	Length	Quality of chain		
1	Н	681	75%	19%	•••
1	Ι	681	75%	18%	• •
1	J	681	74%	19%	• •
1	Κ	681	77%	17%	••
1	L	681	75%	18%	•••



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 65153 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	А	651	Total	С	Ν	0	S	0	0	0
		001	5377	3422	969	961	25	Ŭ		
1	В	645	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0	0
1	D	040	5330	3395	960	952	23	0	0	0
1	С	648	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0	0
1	U	040	5358	3412	966	955	25	0	0	0
1	Л	650	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0	0
	D	050	5373	3420	968	960	25	0	0	0
1	F	661	Total	С	Ν	0	S	0	0	0
	Ľ	001	5450	3466	981	976	27	0	0	0
1	F	657	Total	С	Ν	0	S	0	0	0
	Г	037	5421	3448	976	971	26	0	0	0
1	С	650	Total	С	Ν	0	S	0	0	0
	G	059	5431	3453	978	973	27	0	0	0
1	Ц	661	Total	С	Ν	0	S	0	0	0
	11	001	5450	3466	981	976	27	0	0	0
1	т	660	Total	С	Ν	0	S	0	0	0
1	1	000	5442	3462	979	974	27	0	0	0
1	т	650	Total	С	Ν	0	S	0	0	0
1	J	059	5431	3453	978	973	27	0	0	0
1	TZ IZ	660	Total	С	Ν	Ο	S	0	0	0
	n	000	5442	3462	979	974	27	U	0	U
1	т	650	Total	С	Ν	0	S	0	0	0
		099	5431	3453	978	973	27	U	U	U

• Molecule 1 is a protein called TK receptor.

• Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Cu 2 2	0	0
2	В	2	Total Cu 2 2	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	С	2	Total Cu 2 2	0	0
2	D	2	Total Cu 2 2	0	0
2	Е	2	Total Cu 2 2	0	0
2	F	2	Total Cu 2 2	0	0
2	G	2	Total Cu 2 2	0	0
2	Н	2	Total Cu 2 2	0	0
2	Ι	2	Total Cu 2 2	0	0
2	J	2	Total Cu 2 2	0	0
2	К	2	Total Cu 2 2	0	0
2	L	2	Total Cu 2 2	0	0

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• Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Ato	$\mathbf{ms}$		ZeroOcc	AltConf
3	А	1	Total 4	С 2	O 2	0	0



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

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	31	Total         O           31         31	0	0
4	В	25	Total O 25 25	0	0
4	С	23	TotalO2323	0	0
4	D	13	Total         O           13         13	0	0
4	Е	14	Total O 14 14	0	0
4	F	12	Total         O           12         12	0	0
4	G	8	Total O 8 8	0	0
4	Н	6	Total O 6 6	0	0
4	Ι	8	Total O 8 8	0	0
4	J	6	Total O 6 6	0	0
4	К	1	Total O 1 1	0	0
4	L	18	Total         O           18         18	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. 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. 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: TK receptor





#### 

• Molecule 1: TK receptor



Chain E: 72% 21% ·









#### R638 K639 F643 D654 R680 T681

• Molecule 1: TK receptor



 $\bullet$  Molecule 1: TK receptor



Chain J:





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# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	121.04Å $364.15$ Å $125.52$ Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $118.95^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution(Å)	48.66 - 3.15	Depositor
Resolution (A)	48.61 - 3.15	EDS
% Data completeness	98.7 (48.66 - 3.15)	Depositor
(in resolution range)	$98.1 \ (48.61 - 3.15)$	EDS
$R_{merge}$	0.24	Depositor
R <sub>sym</sub>	0.24	Depositor
$< I/\sigma(I) > 1$	$1.25 (at 3.12 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
D D .	0.269 , $0.310$	Depositor
$n, n_{free}$	0.269 , $0.308$	DCC
$R_{free}$ test set	7921 reflections $(4.90\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	61.6	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32, 21.9	EDS
L-test for $twinning^2$	$<  L  > = 0.42, < L^2 > = 0.25$	Xtriage
	0.046 for l,k,-h-l	
	0.046 for -h-l,k,h	
Estimated twinning fraction	0.387 for h,-k,-h-l	Xtriage
	0.047 for l,-k,h	
	0.047 for -h-l,-k,l	
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	65153	wwPDB-VP
Average B, all atoms $(Å^2)$	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 11.38% 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: EDO, CU

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	B	ond angles
WIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.39	0/5513	0.80	12/7461~(0.2%)
1	В	0.37	0/5465	0.75	3/7397~(0.0%)
1	С	0.37	0/5494	0.78	8/7435~(0.1%)
1	D	0.39	0/5509	0.75	4/7456~(0.1%)
1	Е	0.36	0/5587	0.74	7/7562~(0.1%)
1	F	0.36	0/5557	0.77	9/7522~(0.1%)
1	G	0.34	0/5567	0.67	0/7535
1	Н	0.34	0/5587	0.68	1/7562~(0.0%)
1	Ι	0.35	0/5579	0.72	8/7551~(0.1%)
1	J	0.34	0/5567	0.70	4/7535~(0.1%)
1	Κ	0.33	0/5579	0.67	2/7551~(0.0%)
1	L	0.35	1/5567~(0.0%)	0.71	10/7535~(0.1%)
All	All	0.36	1/66571~(0.0%)	0.73	$68/\overline{90102}\ (0.1\%)$

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	<b>#Planarity outliers</b>
1	А	0	1
1	В	0	1
1	D	0	3
1	Ε	0	3
1	F	0	4
1	G	0	1
1	Н	0	2
1	J	0	2
1	Κ	0	1
1	L	0	2
All	All	0	20



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	216	GLU	CD-OE2	-5.52	1.19	1.25

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	71	MET	CG-SD-CE	10.93	117.69	100.20
1	С	79	PHE	CB-CA-C	10.66	131.72	110.40
1	F	310	ARG	NE-CZ-NH1	9.65	125.12	120.30
1	F	228	ARG	CG-CD-NE	-9.62	91.59	111.80
1	F	247	ARG	CG-CD-NE	-9.34	92.18	111.80

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	60	ARG	Sidechain
1	В	56	ARG	Sidechain
1	D	34	LEU	Mainchain
1	D	473	ARG	Sidechain
1	D	631	ARG	Sidechain

### 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	5377	0	5284	134	3
1	В	5330	0	5242	105	0
1	С	5358	0	5270	128	3
1	D	5373	0	5281	115	1
1	Е	5450	0	5348	134	0
1	F	5421	0	5324	141	0
1	G	5431	0	5334	92	1
1	Н	5450	0	5348	92	1
1	Ι	5442	0	5341	104	0
1	J	5431	0	5334	107	1
1	K	5442	0	5342	102	1



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	5431	0	5333	113	1
2	А	2	0	0	0	0
2	В	2	0	0	0	0
2	С	2	0	0	0	0
2	D	2	0	0	0	0
2	Е	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	Н	2	0	0	0	0
2	Ι	2	0	0	0	0
2	J	2	0	0	0	0
2	Κ	2	0	0	0	0
2	L	2	0	0	0	0
3	А	12	0	18	0	0
3	D	8	0	12	0	0
3	F	4	0	6	0	0
3	Н	4	0	6	0	0
4	А	31	0	0	0	0
4	В	25	0	0	0	0
4	С	23	0	0	1	0
4	D	13	0	0	0	0
4	Е	14	0	0	2	0
4	F	12	0	0	1	0
4	G	8	0	0	0	0
4	Н	6	0	0	0	0
4	Ι	8	0	0	1	0
4	J	6	0	0	1	0
4	Κ	1	0	0	0	0
4	L	18	0	0	1	0
All	All	65153	0	63823	1273	6

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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 10.

The worst 5 of 1273 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)
1:J:208:HIS:HB3	1:J:581:CYS:SG	1.38	1.60
1:A:132:HIS:CG	1:A:222:ILE:HD11	1.41	1.50
1:J:581:CYS:SG	1:J:622:ASN:HB3	1.55	1.46
1:B:28:ASP:OD1	1:B:56:ARG:NH1	1.60	1.33



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:ASP:O	1:D:101:ARG:HG2	1.34	1.27

The worst 5 of 6 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:D:44:GLU:OE2	1:J:444:VAL:CG1[1_655]	1.59	0.61
1:A:47:ASN:OD1	1:C:438:GLN:NE2[1_656]	1.60	0.60
1:G:102:ASN:OD1	1:K:330:ASN:ND2[2_645]	1.95	0.25
1:A:47:ASN:OD1	1:C:438:GLN:CD[1_656]	1.96	0.24
1:H:102:ASN:OD1	1:L:330:ASN:ND2[2_555]	2.03	0.17

### 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	645/681~(95%)	608 (94%)	30 (5%)	7 (1%)	14	48
1	В	639/681~(94%)	602 (94%)	32~(5%)	5(1%)	19	55
1	С	642/681~(94%)	609~(95%)	27 (4%)	6 (1%)	17	53
1	D	644/681~(95%)	610 (95%)	29 (4%)	5 (1%)	19	55
1	E	655/681~(96%)	620 (95%)	30 (5%)	5 (1%)	19	55
1	F	651/681~(96%)	614 (94%)	29 (4%)	8 (1%)	13	46
1	G	653/681~(96%)	615 (94%)	32~(5%)	6 (1%)	17	53
1	Н	655/681~(96%)	616 (94%)	32 (5%)	7 (1%)	14	48
1	Ι	654/681~(96%)	618 (94%)	30 (5%)	6 (1%)	17	53
1	J	653/681~(96%)	614 (94%)	33~(5%)	6 (1%)	17	53
1	K	$65\overline{4}/681~(96\%)$	617 (94%)	29 (4%)	8 (1%)	13	46
1	L	653/681~(96%)	616 (94%)	31 (5%)	6 (1%)	17	53



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Mol	Chain	Analysed	lysed Favoured		Outliers	Percentiles	
All	All	7798/8172~(95%)	7359~(94%)	364 (5%)	75 (1%)	15 51	

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	218	SER
1	В	630	VAL
1	D	614	VAL
1	D	643	PHE
1	Е	217	ALA

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	А	585/610~(96%)	520 (89%)	65 (11%)	(	5	24
1	В	580/610~(95%)	521 (90%)	59~(10%)		7	27
1	С	583/610~(96%)	517 (89%)	66 (11%)	(	5	23
1	D	585/610~(96%)	529~(90%)	56 (10%)	8	3	29
1	Е	594/610~(97%)	529~(89%)	65 (11%)	(	5	24
1	F	591/610~(97%)	535~(90%)	56 (10%)	8	3	30
1	G	592/610~(97%)	541 (91%)	51 (9%)	1	0	35
1	Η	594/610~(97%)	539~(91%)	55~(9%)	ę	)	31
1	Ι	593/610~(97%)	534 (90%)	59 (10%)	8	3	28
1	J	592/610~(97%)	537 (91%)	55~(9%)	(	)	31
1	Κ	593/610~(97%)	540 (91%)	53~(9%)	ę	)	33
1	L	592/610~(97%)	536~(90%)	56 (10%)	8	3	30
All	All	$707\overline{4/7320}~(97\%)$	6378~(90%)	696 (10%)	8	3	28

 $5~{\rm of}~696$  residues with a non-rotameric side chain are listed below:



Mol	Chain	Res	Type
1	Н	616	ASP
1	J	559	ARG
1	Ι	62	ILE
1	Н	614	VAL
1	Ι	618	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
1	Ι	438	GLN
1	Κ	438	GLN
1	Ι	622	ASN
1	J	615	GLN
1	L	86	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)

Of 31 ligands modelled in this entry, 24 are monoatomic - leaving 7 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 Two		Chain	Dec	Link	Bond lengths			Bond angles		
	for Type Chain I	nes	Counts		RMSZ	# Z  > 2	Counts	RMSZ	# Z >2	
3	EDO	А	705	-	$3,\!3,\!3$	0.21	0	$2,\!2,\!2$	0.42	0
3	EDO	Н	703	-	3,3,3	0.18	0	$2,\!2,\!2$	0.33	0
3	EDO	А	703	-	3,3,3	0.25	0	2,2,2	0.42	0
3	EDO	D	703	-	3,3,3	0.60	0	2,2,2	0.60	0
3	EDO	А	704	-	3,3,3	0.36	0	2,2,2	0.55	0
3	EDO	F	703	-	3,3,3	0.08	0	2,2,2	0.16	0
3	EDO	D	704	-	3,3,3	0.25	0	2,2,2	0.48	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
3	EDO	А	705	-	-	0/1/1/1	-
3	EDO	Н	703	-	-	1/1/1/1	-
3	EDO	А	703	-	-	0/1/1/1	-
3	EDO	D	703	-	-	1/1/1/1	-
3	EDO	А	704	-	-	1/1/1/1	-
3	EDO	F	703	-	-	1/1/1/1	-
3	EDO	D	704	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	704	EDO	O1-C1-C2-O2
3	Н	703	EDO	O1-C1-C2-O2
3	D	703	EDO	O1-C1-C2-O2
3	F	703	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

### 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

