

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	1HA3
Title	:	ELONGATION FACTOR TU IN COMPLEX WITH aurodox
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Deposited on	:	2001-03-26
Resolution	:	2.00 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	:	1.8.4, 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

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1 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6828 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	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	201	Total	С	Ν	0	\mathbf{S}	0	0	0
	A	391	3066	1943	529	581	13	0	0	0
1	р	270	Total	С	Ν	0	S	0	10	0
	D	519	2982	1891	519	559	13	0	10	0

• Molecule 1 is a protein called ELONGATION FACTOR TU.

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	6	ILE	VAL	variant	UNP P07157
А	33	PHE	TYR	variant	UNP P07157
А	35	THR	ALA	variant	UNP P07157
А	264	LYS	ARG	variant	UNP P07157
В	6	ILE	VAL	variant	UNP P07157
В	33	PHE	TYR	variant	UNP P07157
В	$\overline{35}$	THR	ALA	variant	UNP P07157
В	264	LYS	ARG	variant	UNP P07157

• Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
0	Δ	1	Total	С	Ν	Ο	Р	0	0
	2 A	1	28	10	5	11	2	0	0
0	В	1	Total	С	Ν	Ο	Р	0	0
	D		28	10	5	11	2	U	

 $\bullet\,$ Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Mg 1 1	0	0
3	В	1	Total Mg 1 1	0	0

• Molecule 4 is N-METHYL KIRROMYCIN (three-letter code: MAU) (formula: $C_{44}H_{62}N_2O_{12}$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	Λ	1	Total	С	Ν	0	0	0	
4	4 A	T	58	44	2	12	0	0	
4	В	1	Total	С	Ν	0	0	0	
4	D	L	58	44	2	12	0	0	

• Molecule 5 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



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



• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	271	Total O 271 271	0	0
6	В	327	Total O 327 327	0	0

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2 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	69.00Å 101.40Å 79.10Å	Deperitor
a, b, c, α , β , γ	90.00° 113.60° 90.00°	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	20.00 - 2.00	Depositor
Resolution (A)	29.81 - 2.00	EDS
% Data completeness	98.9 (20.00-2.00)	Depositor
(in resolution range)	99.0 (29.81-2.00)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	0.07	Depositor
$< I/\sigma(I) > 1$	$3.55 (at 2.00 \text{\AA})$	Xtriage
Refinement program	CNS 1.0	Depositor
D D.	0.191 , 0.221	Depositor
II, II, <i>free</i>	0.186 , 0.183	DCC
R_{free} test set	3377 reflections $(5.07%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	24.2	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	$0.35 \;, 53.3$	EDS
L-test for $twinning^2$	$< L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6828	wwPDB-VP
Average B, all atoms $(Å^2)$	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.28% 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.

3 Model quality (i)

3.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BME, GDP, MG, MAU

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	# Z > 5	RMSZ	# Z > 5	
1	А	0.30	0/3157	0.64	1/4283~(0.0%)	
1	В	0.31	0/3080	0.68	1/4177~(0.0%)	
All	All	0.31	0/6237	0.66	2/8460~(0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	78	SER	N-CA-C	-5.57	95.95	111.00
1	В	78	SER	N-CA-C	-5.51	96.12	111.00

There are no chirality outliers.

There are no planarity outliers.

3.2 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	3066	0	3073	49	0
1	В	2982	0	2999	67	0
2	А	28	0	12	1	0
2	В	28	0	12	2	0
3	А	1	0	0	0	0
3	В	1	0	0	0	0
4	А	58	0	60	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	В	58	0	60	1	0
5	А	4	0	5	3	0
5	В	4	0	5	5	0
6	А	271	0	0	3	0
6	В	327	0	0	2	0
All	All	6828	0	6226	117	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 9.

All (117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:98[B]:GLN:HG3	1:B:241:ARG:HE	1.12	1.09
1:B:285:ASN:HD22	1:B:285:ASN:H	1.22	0.84
1:B:272:MET:HE3	1:B:284:ASP:HB3	1.61	0.82
1:B:98[B]:GLN:HG3	1:B:241:ARG:NE	1.93	0.82
1:B:117:ARG:HG2	1:B:157[A]:LEU:HD11	1.65	0.76
1:B:82:CYS:HA	5:B:482:BME:H12	1.69	0.73
1:B:285:ASN:H	1:B:285:ASN:ND2	1.88	0.71
1:A:224:PRO:HG3	1:A:345:ARG:HD3	1.74	0.70
1:B:228:VAL:HG11	1:B:298:VAL:HG13	1.74	0.68
1:B:334:PHE:HB2	1:B:362:VAL:CG2	2.27	0.65
1:B:100:ASP:O	1:B:129:PRO:HG2	1.97	0.64
1:B:74[A]:LYS:HG2	1:B:75:ARG:HG3	1.78	0.64
1:B:142:ASP:O	1:B:144:PRO:HD3	1.97	0.64
1:A:362:VAL:HG21	1:A:368:VAL:HG21	1.79	0.63
1:B:263[A]:ARG:NH2	1:B:302:GLN:HE22	1.96	0.62
1:A:74:LYS:HG2	1:A:75:ARG:HG3	1.81	0.62
1:B:315:LYS:HB3	1:B:405:GLU:HG2	1.82	0.61
1:A:33:PHE:CZ	1:A:44:VAL:HG13	2.36	0.60
1:B:252:GLU:OE1	1:B:264:LYS:HE2	2.00	0.60
1:B:228:VAL:HG12	1:B:295:ARG:HG3	1.82	0.60
1:A:278:GLN:HB3	6:A:2170:HOH:O	2.02	0.60
1:A:171:ILE:HD12	1:A:171:ILE:N	2.17	0.59
1:A:120:ILE:HD12	1:A:157[B]:LEU:HD22	1.83	0.59
1:B:98[B]:GLN:CG	1:B:241:ARG:HE	2.03	0.59
1:B:5:PHE:HB2	1:B:275:LYS:HB2	1.84	0.59
1:A:100:ASP:O	1:A:129:PRO:HG2	2.03	0.58
1:B:385:ARG:HG2	1:B:399[B]:VAL:HG22	1.85	0.58
1:A:230:THR:N	1:A:295:ARG:HH21	2.01	0.57



A + a 1	Atom 9	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:149:LEU:O	1:A:153:GLU:HG3	2.04	0.57
1:A:120:ILE:CD1	1:A:157[B]:LEU:HD22	2.34	0.57
1:B:274:ARG:HH11	1:B:274:ARG:HG3	1.69	0.57
1:B:117:ARG:HG2	1:B:157[A]:LEU:CD1	2.34	0.56
1:A:231:ILE:CG2	1:A:234:ARG:HD3	2.35	0.56
1:A:80[A]:VAL:HG11	5:A:482:BME:H22	1.87	0.56
1:A:231:ILE:HG21	1:A:234:ARG:HD3	1.87	0.55
1:A:25:THR:HG21	1:A:51:ASP:HB2	1.89	0.55
1:A:19:HIS:ND1	1:A:115:GLN:HB2	2.22	0.54
1:B:285:ASN:HD22	1:B:285:ASN:N	2.00	0.54
1:A:324:LYS:HE2	6:A:2085:HOH:O	2.08	0.53
1:A:124:ARG:HG2	1:A:163:PHE:CE2	2.44	0.52
1:A:268:THR:HG23	1:A:291:ARG:HB2	1.91	0.52
1:B:171:ILE:HD12	1:B:171:ILE:N	2.24	0.52
1:B:80[A]:VAL:CG1	5:B:482:BME:H21	2.39	0.52
1:B:94:THR:O	1:B:98[B]:GLN:NE2	2.42	0.52
1:A:52:LYS:NZ	1:A:65:THR:HA	2.25	0.52
1:B:294:SER:OG	1:B:297:GLU:HG3	2.10	0.51
1:B:389:ARG:HG2	1:B:394:THR:HA	1.92	0.51
1:B:274:ARG:HG3	1:B:274:ARG:NH1	2.25	0.50
1:B:254:GLU:HG3	1:B:307:PRO:HA	1.94	0.49
1:A:268:THR:CG2	1:A:291:ARG:HB2	2.42	0.49
1:B:360:GLU:O	1:B:361:MET:HG3	2.13	0.49
1:A:220:PRO:O	1:A:244:ARG:HG3	2.13	0.48
1:B:272:MET:HE2	1:B:285:ASN:O	2.12	0.48
1:B:92:MET:HG2	1:B:122[A]:LEU:HD23	1.93	0.48
1:A:69:GLU:HB3	1:A:273:HIS:CD2	2.49	0.48
1:B:95:GLY:O	1:B:98[A]:GLN:HG3	2.12	0.48
1:B:317:GLU:HG2	1:B:371:THR:HG22	1.95	0.48
1:B:295:ARG:HH11	1:B:295:ARG:HB2	1.78	0.48
1:B:124:ARG:HG2	1:B:163:PHE:CE2	2.48	0.47
1:A:289:LEU:N	1:A:289:LEU:HD12	2.29	0.47
1:A:138:VAL:HG22	1:A:173:GLY:O	2.15	0.47
1:A:244:ARG:HD3	6:A:2145:HOH:O	2.14	0.47
1:A:291:ARG:HG3	1:A:291:ARG:HH11	1.79	0.47
1:A:230:THR:H	1:A:295:ARG:HH21	1.64	0.46
1:A:69:GLU:HB3	1:A:273:HIS:NE2	2.31	0.46
1:A:291:ARG:O	1:A:293:VAL:HG13	2.16	0.46
1:A:236:THR:HG21	1:A:294:SER:C	2.36	0.46
1:B:228:VAL:CG1	1:B:298:VAL:HG13	2.45	0.46
1:A:222:LEU:HD22	1:A:305:ALA:HB2	1.98	0.45



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:389:ARG:NH2	1:B:392:GLY:HA2	2.32	0.45
1:B:80[A]:VAL:HG11	5:B:482:BME:H21	1.98	0.45
1:B:330:ARG:HD2	6:B:2259:HOH:O	2.17	0.45
1:A:389:ARG:HG2	1:A:394:THR:HA	1.99	0.44
1:B:98[B]:GLN:HG2	1:B:241:ARG:HB3	1.99	0.44
1:A:36:ALA:HA	1:A:42:VAL:HB	1.99	0.44
1:B:137:LYS:HG2	2:B:406:GDP:C6	2.52	0.44
1:B:92:MET:HA	5:B:482:BME:S2	2.57	0.44
1:A:294:SER:C	1:A:296:GLU:H	2.21	0.44
1:A:176:LEU:O	1:A:180:GLU:HG3	2.18	0.44
1:B:404:LEU:O	1:B:405:GLU:HB3	2.18	0.44
1:A:39:ASN:ND2	1:A:71:GLU:HG3	2.33	0.43
1:B:149:LEU:O	1:B:153:GLU:HG3	2.18	0.43
1:A:80[A]:VAL:CG1	5:A:482:BME:H22	2.48	0.43
1:B:263[A]:ARG:HH11	1:B:263[A]:ARG:HG2	1.83	0.43
1:A:137:LYS:HG2	2:A:406:GDP:C6	2.53	0.43
1:B:117:ARG:NH1	1:B:157[A]:LEU:HD13	2.33	0.43
1:B:220:PRO:O	1:B:244:ARG:HG3	2.19	0.43
1:A:92:MET:SD	1:A:122[A]:LEU:HD23	2.59	0.43
1:A:194:GLU:O	1:A:198:LYS:HG2	2.19	0.43
1:B:334:PHE:HB2	1:B:362:VAL:HG23	2.00	0.43
1:B:117:ARG:CZ	1:B:157[A]:LEU:HD13	2.49	0.43
1:B:20:VAL:O	1:B:21:ASP:HB2	2.19	0.42
1:A:92:MET:HA	5:A:482:BME:S2	2.59	0.42
1:A:385:ARG:HG2	1:A:399[B]:VAL:HG22	2.01	0.42
1:A:89:ILE:HG23	1:A:90:LYS:N	2.35	0.42
1:A:254:GLU:HG3	1:A:307:PRO:HA	2.00	0.42
1:B:121:LEU:O	1:B:125:GLN:HG3	2.19	0.42
1:B:80[A]:VAL:HG12	5:B:482:BME:H21	2.01	0.42
1:B:334:PHE:HB2	1:B:362:VAL:HG22	2.01	0.42
1:A:171:ILE:N	1:A:171:ILE:CD1	2.83	0.42
1:B:263[A]:ARG:NH1	1:B:297:GLU:O	2.50	0.42
1:B:74[A]:LYS:HG2	1:B:75:ARG:CG	2.45	0.41
1:B:295:ARG:HH11	1:B:295:ARG:CB	2.33	0.41
1:B:389:ARG:HH21	1:B:392:GLY:HA2	1.85	0.41
1:B:117:ARG:NH1	1:B:157[A]:LEU:CD1	2.83	0.41
1:B:354:GLN:NE2	6:B:2273:HOH:O	2.48	0.41
1:B:317:GLU:CG	1:B:371:THR:HG22	2.51	0.41
1:A:39:ASN:HA	1:A:40:PRO:HD2	1.97	0.41
1:B:317:GLU:HB2	1:B:402:LYS:HB3	2.03	0.41
1:B:333:GLY:H	1:B:361:MET:HE3	1.86	0.41



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:408:MAU:HC32	4:B:408:MAU:H441	1.97	0.41
1:B:137:LYS:HE2	2:B:406:GDP:C4	2.56	0.40
1:B:295:ARG:CB	1:B:295:ARG:NH1	2.84	0.40
1:B:263[A]:ARG:HH21	1:B:302:GLN:HE22	1.66	0.40

There are no symmetry-related clashes.

3.3 Torsion angles (i)

3.3.1 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	Percentiles
1	А	395/405~(98%)	385~(98%)	9~(2%)	1 (0%)	41 37
1	В	385/405~(95%)	376~(98%)	9(2%)	0	100 100
All	All	780/810~(96%)	761 (98%)	18 (2%)	1 (0%)	51 49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	292	GLY

3.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	337/339~(99%)	334~(99%)	3~(1%)	78 83



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	В	328/339~(97%)	322~(98%)	6(2%)	59 63
All	All	665/678~(98%)	656~(99%)	9 (1%)	71 72

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	21	ASP
1	А	44	VAL
1	А	384	LEU
1	В	16	THR
1	В	121	LEU
1	В	226	GLU
1	В	263[A]	ARG
1	В	263[B]	ARG
1	В	285	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	39	ASN
1	А	278	GLN
1	В	91	ASN
1	В	278	GLN
1	В	285	ASN

3.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

3.5 Carbohydrates (i)

There are no monosaccharides in this entry.



3.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	Dec	Bond lengths			Bond angles			
	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
5	BME	А	482	1	3,3,3	0.34	0	1,2,2	0.12	0
4	MAU	А	408	-	57,60,60	3.13	12 (21%)	65,86,86	1.49	10 (15%)
2	GDP	В	406	3	24,30,30	1.01	1 (4%)	30,47,47	0.70	0
4	MAU	В	408	-	57,60,60	3.17	13 (22%)	65,86,86	1.50	13 (20%)
5	BME	В	482	1	3,3,3	0.39	0	1,2,2	0.24	0
2	GDP	А	406	3	24,30,30	1.01	1 (4%)	30,47,47	0.73	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
5	BME	А	482	1	-	0/1/1/1	-
4	MAU	А	408	-	-	2/54/98/98	0/3/3/3
2	GDP	В	406	3	-	2/12/32/32	0/3/3/3
4	MAU	В	408	-	-	3/54/98/98	0/3/3/3
5	BME	В	482	1	-	0/1/1/1	-
2	GDP	A	406	3	-	3/12/32/32	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
4	А	408	MAU	O18-C17	-15.82	1.20	1.44
4	В	408	MAU	O18-C17	-15.71	1.20	1.44
4	В	408	MAU	O30-C30	-13.50	1.15	1.42
4	А	408	MAU	O30-C30	-13.45	1.15	1.42
4	В	408	MAU	C22-C21	4.30	1.37	1.33
4	А	408	MAU	C27-N26	4.07	1.42	1.33



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	В	408	MAU	C27-N26	4.00	1.42	1.33
4	А	408	MAU	C22-C21	3.82	1.37	1.33
4	В	408	MAU	C29-C28	3.60	1.61	1.54
4	В	408	MAU	C45-C28	3.59	1.60	1.53
4	В	408	MAU	O29-C29	3.39	1.46	1.40
4	А	408	MAU	O29-C29	3.18	1.46	1.40
4	А	408	MAU	C45-C28	3.17	1.59	1.53
4	А	408	MAU	C29-C28	3.17	1.61	1.54
4	В	408	MAU	C32-C33	-2.79	1.51	1.55
4	В	408	MAU	C19-C17	2.70	1.60	1.54
2	А	406	GDP	C8-N7	-2.49	1.30	1.35
4	А	408	MAU	C42-C19	2.46	1.58	1.53
4	В	408	MAU	C42-C19	2.37	1.58	1.53
2	В	406	GDP	C8-N7	-2.32	1.31	1.35
4	А	408	MAU	C16-C17	2.19	1.57	1.52
4	А	408	MAU	C19-C17	2.17	1.59	1.54
4	В	408	MAU	C6-C5	2.15	1.42	1.38
4	В	408	MAU	C16-C17	2.12	1.57	1.52
4	А	408	MAU	C32-C33	-2.09	1.52	1.55
4	А	408	MAU	C6-C5	2.08	1.42	1.38
4	В	408	MAU	C20-C21	2.06	1.54	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
4	А	408	MAU	C29-C30-C31	-4.51	104.69	110.66
4	В	408	MAU	C29-C30-C31	-3.93	105.46	110.66
4	А	408	MAU	O18-C17-C16	3.69	111.20	104.27
4	В	408	MAU	O18-C17-C16	3.56	110.96	104.27
4	В	408	MAU	C44-C21-C20	2.98	120.83	115.68
4	В	408	MAU	C3-C2-N1	2.97	120.27	116.66
4	А	408	MAU	C11-C10-C9	-2.94	117.46	123.47
4	В	408	MAU	O29-C29-O34	-2.93	105.31	110.21
4	В	408	MAU	C11-C10-C9	-2.91	117.51	123.47
4	А	408	MAU	C3-C2-N1	2.85	120.12	116.66
4	А	408	MAU	C23-C22-C21	-2.83	123.16	127.32
4	В	408	MAU	C45-C28-C27	2.74	112.73	108.86
4	А	408	MAU	C44-C21-C20	2.74	120.41	115.68
4	А	408	MAU	O29-C29-O34	-2.73	105.64	110.21
4	А	408	MAU	C45-C28-C27	2.53	112.44	108.86
4	В	408	MAU	C16-C15-C14	-2.51	98.88	101.87
4	В	408	MAU	C23-C22-C21	-2.50	123.65	127.32



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	В	408	MAU	C17-C19-C20	-2.33	105.70	111.97
4	А	408	MAU	C14-C13-C12	-2.29	121.13	125.61
4	В	408	MAU	O34-C29-C28	2.19	110.19	104.46
4	В	408	MAU	C14-C13-C12	-2.15	121.39	125.61
4	В	408	MAU	C22-C23-C24	-2.10	118.70	123.63
4	А	408	MAU	C16-C15-C14	-2.08	99.38	101.87

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
2	А	406	GDP	PA-O3A-PB-O2B
2	А	406	GDP	PA-O3A-PB-O3B
2	В	406	GDP	PA-O3A-PB-O3B
4	А	408	MAU	C36-C37-C38-C39
4	В	408	MAU	C36-C37-C38-C39
2	В	406	GDP	PA-O3A-PB-O1B
4	В	408	MAU	C2-C3-C7-O7
2	А	406	GDP	PA-O3A-PB-O1B
4	А	408	MAU	C27-C28-C45-C46
4	В	408	MAU	C27-C28-C45-C46

All (10) torsion outliers are listed below:

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	А	482	BME	3	0
2	В	406	GDP	2	0
4	В	408	MAU	1	0
5	В	482	BME	5	0
2	А	406	GDP	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.









3.7 Other polymers (i)

There are no such residues in this entry.

3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



4 Fit of model and data (i)

4.1 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	391/405~(96%)	-0.11	23 (5%) 22 21	20, 29, 55, 77	0
1	В	379/405~(93%)	-0.39	6 (1%) 72 70	17, 25, 40, 76	0
All	All	770/810~(95%)	-0.25	29 (3%) 40 39	17, 27, 49, 77	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	48	GLY	6.2
1	А	52	LYS	6.1
1	А	47	TYR	5.7
1	А	50	ILE	5.2
1	А	40	PRO	4.9
1	А	291	ARG	4.6
1	А	44	VAL	4.5
1	А	49	ASP	4.1
1	А	46	ASP	3.9
1	А	146	LEU	3.7
1	А	51	ASP	3.4
1	А	232	THR	3.2
1	А	142	ASP	3.2
1	А	3	GLY	3.1
1	В	41	ASN	3.0
1	А	42	VAL	3.0
1	В	3	GLY	3.0
1	А	65	THR	2.9
1	А	358	GLY	2.9
1	В	40	PRO	2.9
1	А	234	ARG	2.9
1	В	142	ASP	2.8
1	A	43	GLU	2.7
1	В	66	ALA	2.3



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Mol	Chain	Res	Type	RSRZ
1	А	231	ILE	2.3
1	В	295	ARG	2.1
1	А	145	GLU	2.1
1	А	45	LYS	2.0
1	А	233	GLY	2.0

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

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

4.3 Carbohydrates (i)

There are no monosaccharides in this entry.

4.4 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	${f B} ext{-factors}({ m \AA}^2)$	Q < 0.9
4	MAU	В	408	58/58	0.93	0.11	18,24,31,33	0
4	MAU	А	408	58/58	0.94	0.10	$19,\!25,\!32,\!35$	0
5	BME	В	482	4/4	0.94	0.12	30,30,35,37	0
5	BME	А	482	4/4	0.95	0.11	29,32,36,42	0
2	GDP	А	406	28/28	0.99	0.06	19,26,28,31	0
2	GDP	В	406	28/28	0.99	0.06	18,23,27,32	0
3	MG	А	407	1/1	0.99	0.03	22,22,22,22	0
3	MG	В	407	1/1	0.99	0.03	22,22,22,22	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.











4.5 Other polymers (i)

There are no such residues in this entry.

