

Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2021 - 10.55 am BST

PDB ID : 700P

Title : Crystal structure of the human METTL3-METTL14 complex bound to Com-

pound 10 (ADO AD 022)

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Deposited on : 2021-03-26

Resolution : 2.70 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 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)

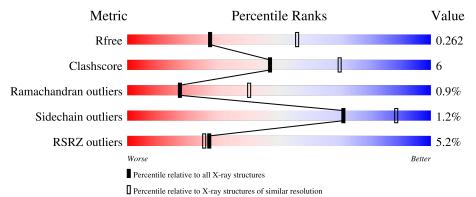
Validation Pipeline (wwPDB-VP) : 2.23.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{A})}) \end{array}$
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	A	246	67%	15%	18%			
2	В	290	72%	10%	17%			



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3492 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.

• Molecule 1 is a protein called N6-adenosine-methyltransferase catalytic subunit.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	202	Total	С	N	О	S	0	0	0
1	A	202	1572	1010	273	280	9	0	U	

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	MET	-	initiating methionine	UNP Q86U44
A	336	GLY	_	expression tag	UNP Q86U44
A	337	HIS	_	expression tag	UNP Q86U44
A	338	HIS	_	expression tag	UNP Q86U44
A	339	HIS	-	expression tag	UNP Q86U44
A	340	HIS	_	expression tag	UNP Q86U44
A	341	HIS	-	expression tag	UNP Q86U44
A	342	HIS	-	expression tag	UNP Q86U44
A	343	SER	-	expression tag	UNP Q86U44
A	344	SER	-	expression tag	UNP Q86U44
A	345	GLY	-	expression tag	UNP Q86U44
A	346	ARG	-	expression tag	UNP Q86U44
A	347	GLU	-	expression tag	UNP Q86U44
A	348	ASN	-	expression tag	UNP Q86U44
A	349	LEU	-	expression tag	UNP Q86U44
A	350	TYR	-	expression tag	UNP Q86U44
A	351	PHE	-	expression tag	UNP Q86U44
A	352	GLN	=	expression tag	UNP Q86U44
A	353	GLY	-	expression tag	UNP Q86U44

• Molecule 2 is a protein called N6-adenosine-methyltransferase non-catalytic subunit.

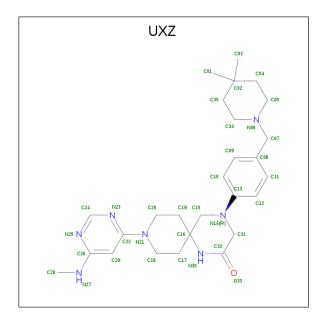
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	241	Total 1848	C 1188	N 314	O 334	S 12	0	0	0



There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference	
В	106	MET	-	initiating methionine	UNP Q9HCE5	

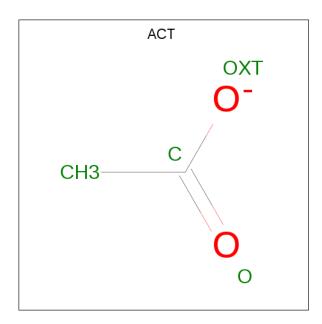
• Molecule 3 is 4-[4-[(4,4-dimethylpiperidin-1-yl)methyl]phenyl]-9-[6-(methylamino)pyrimidin-4-yl]-1,4,9-triazaspiro[5.5]undecan-2-one (three-letter code: UXZ) (formula: $C_{27}H_{39}N_7O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	${f Atoms}$				ZeroOcc	${f AltConf}$
3	A	1	Total 35	C 27		O 1	0	0

• Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	В	1	Total 4	C 2	O 2	0	0

• Molecule 5 is water.

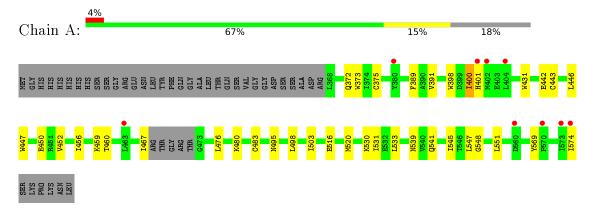
Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
5	A	11	Total O 11 11	0	0
5	В	22	Total O 22 22	0	0



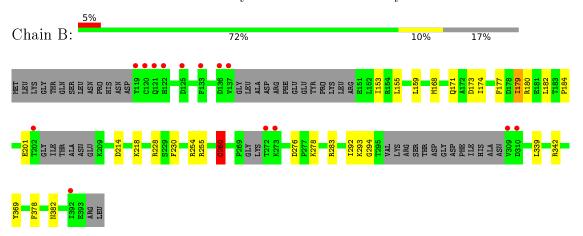
3 Residue-property plots (i)

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: N6-adenosine-methyltransferase catalytic subunit



• Molecule 2: N6-adenosine-methyltransferase non-catalytic subunit





4 Data and refinement statistics (i)

Property	Value	Source		
Space group	P 32 2 1	Depositor		
Cell constants	$64.15 \text{\AA} 64.15 \text{Å} 225.41 \text{Å}$	Depositor		
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor		
Resolution (Å)	44.67 - 2.70	Depositor		
resolution (A)	44.67 - 2.70	EDS		
% Data completeness	99.8 (44.67-2.70)	Depositor		
(in resolution range)	99.8 (44.67-2.70)	EDS		
R_{merge}	(Not available)	Depositor		
R_{sym}	(Not available)	Depositor		
$< I/\sigma(I) > 1$	1.96 (at 2.69Å)	Xtriage		
Refinement program	PHENIX 1.19.1_4122	Depositor		
D D.	0.202 , 0.263	Depositor		
R, R_{free}	0.201 , 0.262	DCC		
R_{free} test set	782 reflections (5.02%)	wwPDB-VP		
Wilson B-factor (Å ²)	58.9	Xtriage		
Anisotropy	0.012	Xtriage		
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33 , 48.4	EDS		
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage		
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage		
F_o, F_c correlation	0.94	EDS		
Total number of atoms	3492	wwPDB-VP		
Average B, all atoms (Å ²)	55.0	wwPDB-VP		

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.

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



 $^{^{1}}$ 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: ACT, UXZ

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).

Mol	Chain	Boı	nd lengths	Bond angles		
Moi Chain		RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.45	0/1614	0.66	0/2202	
2	В	0.46	1/1895 (0.1%)	0.66	1/2579 (0.0%)	
All	All	0.46	$1/3509 \ (0.0\%)$	0.66	1/4781 (0.0%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$Ideal(\AA)$
2	В	260	CYS	CB-SG	-5.24	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	276	ASP	CB-CG-OD1	5.81	123.53	118.30

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	A	1572	0	1487	26	0
2	В	1848	0	1700	18	0
3	A	35	0	0	0	0
4	В	4	0	3	1	0

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Mol	Chain	Non-H	$\mathbf{H}(\mathbf{model})$	H(added)	Clashes	Symm-Clashes
5	A	11	0	0	0	0
5	В	22	0	0	1	0
All	All	3492	0	3190	41	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 6.

All (41) 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	${ m distance}({ m \AA})$	$ \text{overlap } (\text{\AA})$
1:A:400:ILE:HG13	1:A:401:HIS:H	1.38	0.88
2:B:382:ASN:O	5:B:501:HOH:O	2.09	0.69
2:B:255:ARG:HB2	4:B:401:ACT:H3	1.77	0.67
1:A:373:TRP:HB2	1:A:551:LEU:HD13	1.78	0.65
1:A:533:LEU:HD23	1:A:547:LEU:HD12	1.80	0.62
1:A:450:GLU:OE2	2:B:278:LYS:NZ	2.33	0.60
1:A:391:VAL:HB	1:A:530:LYS:HG2	1.86	0.57
2:B:184:PRO:HG2	2:B:342:ARG:HD2	1.87	0.56
1:A:442:GLU:O	1:A:446:LEU:HG	2.06	0.56
1:A:452:VAL:O	2:B:283:ARG:NH2	2.40	0.54
1:A:389:PHE:CE2	1:A:531:ILE:HB	2.44	0.53
1:A:569:TYR:CE1	1:A:574:ILE:HA	2.44	0.52
2:B:228:ARG:HA	2:B:293:LYS:O	2.10	0.52
1:A:398:TRP:HB2	1:A:400:ILE:HG23	1.92	0.51
1:A:431:TRP:CE3	1:A:483:CYS:HB2	2.46	0.50
2:B:168:MET:HE3	2:B:369:TYR:HA	1.93	0.50
2:B:342:ARG:HG2	2:B:378:PHE:CZ	2.46	0.49
1:A:480:LYS:HE2	2:B:260:CYS:HB2	1.93	0.49
1:A:456:ILE:O	1:A:456:ILE:HG13	2.13	0.47
2:B:230:PHE:CE2	2:B:292:ILE:HD12	2.50	0.46
1:A:539:ASN:O	1:A:541:GLN:HG2	2.15	0.46
2:B:214:ASP:O	2:B:218:LYS:HG3	2.16	0.46
1:A:372:GLN:HB2	1:A:545:ILE:HG12	1.97	0.46
1:A:443:CYS:HB3	1:A:447:TRP:CZ2	2.52	0.45
1:A:400:ILE:CG1	1:A:401:HIS:H	2.14	0.44
1:A:516:GLU:O	1:A:520:MET:HG3	2.18	0.43
2:B:254:ARG:NH2	2:B:294:GLY:O	2.51	0.43
1:A:459:LYS:HB2	1:A:459:LYS:HE2	1.73	0.43
2:B:179:ILE:H	2:B:179:ILE:HG12	1.41	0.43
1:A:495:ASN:HB3	1:A:498:LEU:HD13	1.99	0.42
2:B:230:PHE:CZ	2:B:339:LEU:HD22	2.54	0.42

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Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	Clash overlap (Å)
1:A:400:ILE:HD13	1:A:400:ILE:HG21	1.80	0.42
2:B:182:LEU:HD23	2:B:182:LEU:HA	1.87	0.42
1:A:375:CYS:HA	1:A:548:GLY:O	2.19	0.41
1:A:503:ILE:HD11	1:A:520:MET:SD	2.60	0.41
1:A:569:TYR:HE1	1:A:574:ILE:HA	1.85	0.41
1:A:460:THR:O	1:A:467:ILE:HD11	2.21	0.41
2:B:155:LEU:O	2:B:159:LEU:HG	2.21	0.41
2:B:174:ILE:HA	2:B:177:PHE:HB3	2.02	0.41
1:A:476:LEU:HD23	1:A:476:LEU:HA	1.91	0.40
2:B:230:PHE:CE1	2:B:339:LEU:HD22	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	\mathbf{ntiles}
1	A	198/246~(80%)	185 (93%)	12 (6%)	1 (0%)	29	54
2	В	$231/290 \ (80\%)$	220 (95%)	8 (4%)	3 (1%)	12	30
All	All	429/536~(80%)	405 (94%)	20 (5%)	4 (1%)	17	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	201	GLU
1	A	400	ILE
2	В	180	ARG
2	В	153	ILE



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	Percentiles		
1	A	$161/215 \; (75\%)$	161 (100%)	0	100 100		
2	В	183/259 (71%)	179 (98%)	4 (2%)	52 79		
All	All	344/474 (73%)	340 (99%)	4 (1%)	71 88		

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	171	GLN
2	В	173	ASP
2	В	179	ILE
2	В	260	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	${f Res}$	\mathbf{Type}
2	В	128	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)

2 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).

Mol Type		Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain De	Res	Link	Bond lengths			В	ond ang	les
MIOI	Type	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2										
3	UXZ	A	601	-	38,39,39	1.78	10 (26%)	46,57,57	1.87	8 (17%)										
4	ACT	В	401	-	1,3,3	8.51	1 (100%)	0,3,3	0.00	-										

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	${f Torsions}$	Rings
3	UXZ	A	601	-	-	2/14/52/52	0/4/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$Ideal(\AA)$
4	В	401	ACT	СН3-С	8.51	1.59	1.48
3	A	601	UXZ	C32-N30	5.78	1.42	1.34
3	A	601	UXZ	C19-C16	-4.22	1.46	1.54
3	A	601	UXZ	C31-C32	3.48	1.55	1.51
3	A	601	UXZ	C26-N27	2.91	1.42	1.36
3	A	601	UXZ	C24-N23	2.28	1.38	1.33
3	A	601	UXZ	C22-N21	2.18	1.42	1.37
3	A	601	UXZ	C19-C20	2.18	1.57	1.52
3	A	601	UXZ	C20-N21	2.18	1.50	1.46
3	A	601	UXZ	C18-N21	-2.14	1.43	1.46
3	A	601	UXZ	C09-C10	2.01	1.42	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	${f Res}$	Type	${f Atoms}$	${f Z}$	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^o)$
3	A	601	UXZ	C19-C16-C15	5.64	121.27	110.62

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
3	A	601	UXZ	C28-N27-C26	4.32	126.67	122.97
3	A	601	UXZ	O33-C32-N30	-4.18	115.99	121.54
3	A	601	UXZ	C08-C07-N06	-3.91	105.53	113.12
3	A	601	UXZ	C04-C05-N06	-3.69	107.59	111.23
3	A	601	UXZ	C18-N21-C20	3.17	118.51	111.52
3	A	601	UXZ	C19-C20-N21	2.90	115.47	110.34
3	A	601	UXZ	C29-C22-N21	-2.24	119.63	122.29

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	UXZ	C29-C26-N27-C28
3	A	601	UXZ	N25-C26-N27-C28

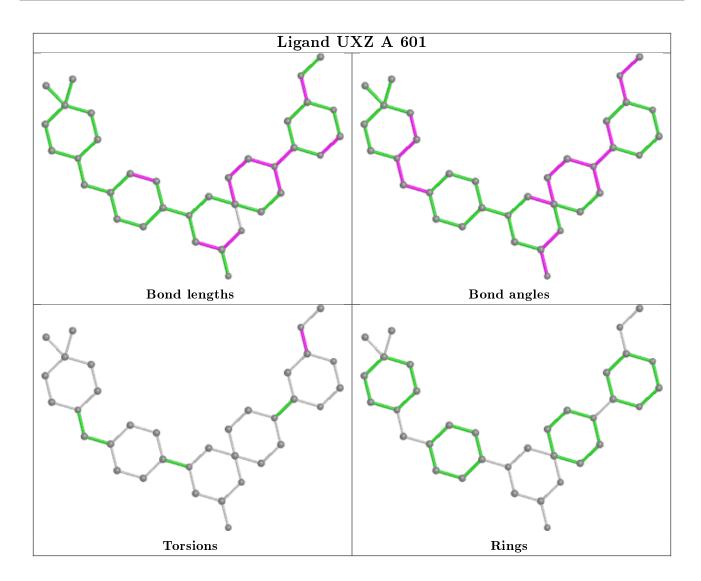
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	401	ACT	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 $>$	#RS	$\mathbf{RZ}>$	>2	$OWAB(A^2)$	Q < 0.9
1	A	$202/246 \ (82\%)$	0.03	9 (4%)	33	31	38, 56, 87, 106	0
2	В	241/290 (83%)	0.03	14 (5%)	23	22	32, 48, 92, 113	0
All	All	443/536 (82%)	0.03	23 (5%)	27	25	32, 53, 91, 113	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	272	THR	5.9
1	A	402	MET	4.4
2	В	137	VAL	4.2
2	В	310	ASP	4.0
2	В	309	VAL	3.8
2	В	120	CYS	3.6
2	В	136	ASP	3.3
2	В	121	GLN	3.2
1	A	570	PRO	3.2
2	В	119	TYR	3.1
2	В	392	ILE	3.1
2	В	202	THR	3.1
2	В	122	HIS	3.0
1	A	574	ILE	3.0
1	A	573	ILE	2.9
1	A	401	HIS	2.8
2	В	273	LYS	2.4
1	A	463	LEU	2.4
1	A	380	TYR	2.3
1	A	560	ASP	2.2
2	В	133	PHE	2.2
2	В	125	ASP	2.0
1	A	404	LEU	2.0



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	${f B-factors}({f A}^2)$	Q<0.9
3	UXZ	A	601	35/35	0.93	0.19	49,53,61,66	0
4	ACT	В	401	4/4	0.97	0.22	46,46,47,50	0

6.5 Other polymers (i)

There are no such residues in this entry.

