

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

#### Jun 3, 2024 – 09:32 PM EDT

PDB ID Title		9BBH Co-crystal structure of human DDB1 bound to fragment UB028670
11016	·	Co-crystal structure of numan DDB1 bound to nagment OD020070
Authors	:	Zeng, H.; Dong, A.; Frommlet, A.; Seitova, A.; Loppnau, P.; Ackloo, S.; Arrow-
		smith, C.H.; Edwards, A.M.; Halabelian, L.; Structural Genomics Consortium
		(SGC)
Deposited on		
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 (i)) were used in the production of this report:

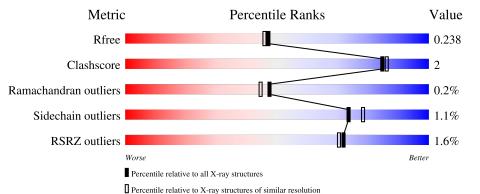
MolProbity		4.02b-467
•		
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

## 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 2.00 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	1142	<sup>2%</sup> 90%	7%	·



#### 9BBH

## 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9333 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.

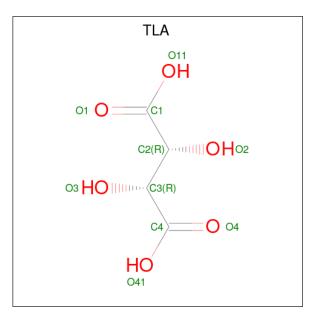
• Molecule 1 is a protein called DNA damage-binding protein 1.

Mo	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	1104	Total 8626	C 5474	N 1451	O 1651	S 50	0	16	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-1	GLY	-	expression tag	UNP Q16531
А	0	SER	-	expression tag	UNP Q16531

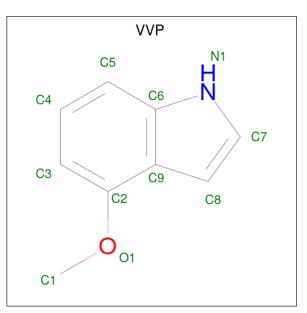
• Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula:  $C_4H_6O_6$ ).



Mo	l	Chain	Residues	Atoms	ZeroOcc	AltConf
2		А	1	Total         C         O           10         4         6	0	0
2		А	1	Total         C         O           10         4         6	0	0

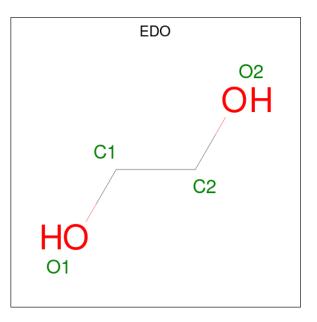


• Molecule 3 is 4-methoxy-1H-indole (three-letter code: VVP) (formula: C<sub>9</sub>H<sub>9</sub>NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total C N O 11 9 1 1	0	0
3	А	1	Total C N O 11 9 1 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	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 5 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	5	Total X 5 5	0	0

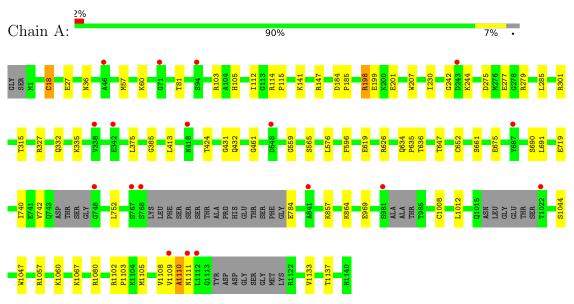
• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	642	Total O 652 652	0	10



## 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: DNA damage-binding protein 1



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	62.92Å 125.27Å 168.53Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	46.82 - 2.00	Depositor
Resolution (A)	46.77 - 2.00	EDS
% Data completeness	99.3 (46.82-2.00)	Depositor
(in resolution range)	99.3 (46.77 - 2.00)	EDS
R <sub>merge</sub>	0.11	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.55 (at 2.00 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
D D.	0.188 , $0.232$	Depositor
$R, R_{free}$	0.197 , $0.238$	DCC
$R_{free}$ test set	4384 reflections $(4.86%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	23.4	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , $48.8$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9333	wwPDB-VP
Average B, all atoms $(Å^2)$	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.34% 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: TLA, VVP, UNX, EDO

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		lengths		ond angles
	ol Chain $]$	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.42	0/8781	0.66	3/11917~(0.0%)

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	# Planarity outliers	
1	А	0	6	

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	57	MET	CG-SD-CE	6.23	110.17	100.20
1	А	18	CYS	CB-CA-C	5.94	122.27	110.40
1	А	327	ARG	CB-CA-C	-5.08	100.25	110.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	103	ARG	Sidechain
1	А	1080	ARG	Sidechain
1	А	147	ARG	Sidechain
1	А	198[A]	ARG	Sidechain
1	А	332	GLN	Peptide
1	А	626	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	8626	0	8459	40	0
2	А	20	0	8	0	0
3	А	22	0	0	0	0
4	А	8	0	11	0	0
5	А	5	0	0	0	0
6	А	652	0	0	5	0
All	All	9333	0	8478	40	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 2.

All (40) 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:A:114:ARG:O	6:A:1301:HOH:O	2.00	0.80
1:A:275:ASP:OD2	1:A:279[B]:ARG:HD3	1.82	0.80
1:A:1105:MET:O	1:A:1109:VAL:HG23	1.95	0.67
1:A:413:LEU:HB3	1:A:424:THR:HB	1.77	0.67
1:A:740:ILE:HG21	1:A:784:GLU:HA	1.78	0.66
1:A:207:TRP:HB3	1:A:242:GLY:HA2	1.81	0.63
1:A:647:THR:HG23	6:A:1819:HOH:O	2.01	0.61
1:A:301:ARG:NH1	6:A:1305:HOH:O	2.32	0.61
1:A:112:ILE:O	6:A:1302:HOH:O	2.17	0.59
1:A:596:PHE:HB3	1:A:661:SER:HB2	1.89	0.55
1:A:742:VAL:HG13	1:A:752:LEU:HD21	1.88	0.54
1:A:1102:ARG:N	1:A:1103:PRO:CD	2.72	0.52
1:A:647:THR:HG22	6:A:1808:HOH:O	2.11	0.50
1:A:413:LEU:CD1	1:A:461:GLY:HA2	2.44	0.48
1:A:740:ILE:CG2	1:A:784:GLU:HA	2.44	0.47
1:A:690:SER:C	1:A:691:LEU:HD12	2.35	0.47
1:A:431:GLY:C	1:A:432:GLN:HG2	2.36	0.45
1:A:576:LEU:C	1:A:576:LEU:HD13	2.36	0.45
1:A:385:GLY:HA3	1:A:719:GLU:O	2.17	0.45
1:A:1133:VAL:O	1:A:1137:THR:HG23	2.17	0.45
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.47	0.44

Continued on next page...



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:1057:ARG:HD3	1:A:1108:VAL:O	2.18	0.43
1:A:1102:ARG:N	1:A:1103:PRO:HD2	2.34	0.43
1:A:18:CYS:SG	1:A:315:THR:HG23	2.59	0.43
1:A:230:ILE:HD11	1:A:285:LEU:HD21	2.01	0.42
1:A:413:LEU:HD13	1:A:461:GLY:HA2	2.02	0.42
1:A:634:GLN:HB3	1:A:635:PRO:HD2	2.01	0.42
1:A:634:GLN:NE2	1:A:675:GLU:OE2	2.44	0.42
1:A:141:LYS:HB2	1:A:141:LYS:HE2	1.83	0.42
1:A:60:LYS:O	1:A:81:THR:HA	2.20	0.41
1:A:1008[A]:CYS:O	1:A:1008[A]:CYS:SG	2.78	0.41
1:A:105:HIS:CE1	1:A:1067:LYS:HD2	2.55	0.41
1:A:199:GLU:O	1:A:201[B]:GLU:HG2	2.19	0.41
1:A:636:THR:HA	1:A:652:CYS:O	2.21	0.41
1:A:375:LEU:HB2	1:A:1012:LEU:HD21	2.02	0.41
1:A:285:LEU:N	1:A:285:LEU:HD12	2.36	0.40
1:A:1110:ALA:O	1:A:1111:ASN:CB	2.68	0.40
1:A:559:GLY:HA2	1:A:565:SER:O	2.21	0.40
1:A:1044:SER:HG	1:A:1047:TRP:HD1	1.69	0.40
1:A:277:GLU:OE1	1:A:279[A]:ARG:NH1	2.55	0.40

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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	Percentiles
1	А	1108/1142~(97%)	1076 (97%)	30 (3%)	2~(0%)	47 44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	1110	ALA
1	А	36	ASN



#### 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	А	941/1000~(94%)	929~(99%)	12 (1%)	69 74

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	27	GLU
1	А	115	PRO
1	А	198[A]	ARG
1	А	198[B]	ARG
1	А	244	LYS
1	А	335[A]	LYS
1	А	335[B]	LYS
1	А	619	GLU
1	А	857	LYS
1	А	864	LYS
1	А	969	GLU
1	А	1060	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	105	HIS
1	А	290	GLN
1	А	418	ASN
1	А	677	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 11 ligands modelled in this entry, 5 are unknown - 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).

Mol	Turne	Chain	Res	Link	Bo	ond leng	ths	Bond angles		
Mol Type	Ullain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
2	TLA	А	1202	-	$9,\!9,\!9$	1.01	0	12,12,12	1.04	0
4	EDO	А	1206	-	3,3,3	0.78	0	2,2,2	0.31	0
4	EDO	А	1205	-	$3,\!3,\!3$	1.34	1 (33%)	$2,\!2,\!2$	0.15	0
3	VVP	А	1204	-	10,12,12	0.77	0	13,16,16	0.66	0
3	VVP	А	1203	-	$10,\!12,\!12$	0.64	0	13, 16, 16	0.67	0
2	TLA	А	1201	-	$9,\!9,\!9$	1.15	1 (11%)	$12,\!12,\!12$	0.97	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
2	TLA	А	1202	-	-	0/12/12/12	-
4	EDO	А	1206	-	-	1/1/1/1	-
4	EDO	А	1205	-	-	1/1/1/1	-
3	VVP	А	1204	-	-	0/2/2/2	0/2/2/2
3	VVP	А	1203	-	-	1/2/2/2	0/2/2/2
2	TLA	А	1201	-	-	0/12/12/12	-

All (2) bond length outliers are listed below:

Mo	l Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	TLA	O1-C1	2.17	1.28	1.22
4	A	1205	EDO	O2-C2	-2.15	1.31	1.42



There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

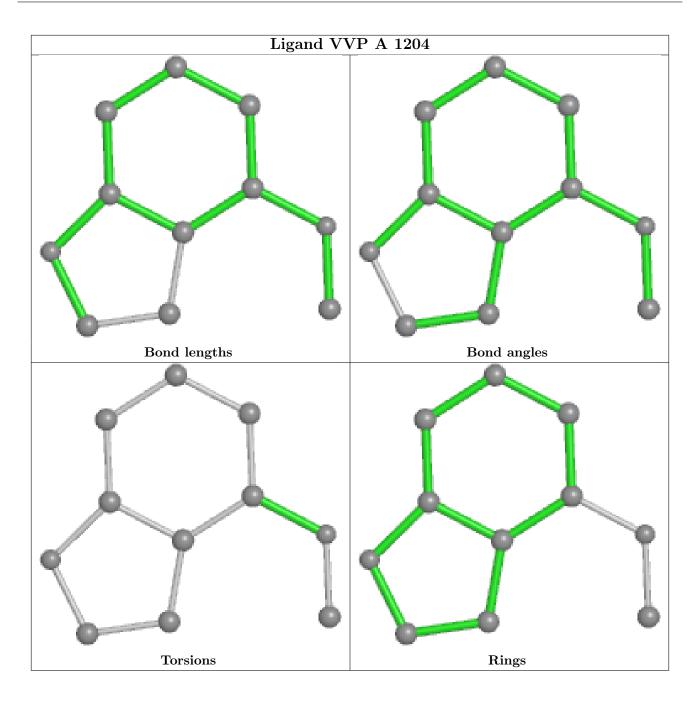
Mol	Chain	Res	Type	Atoms
4	А	1205	EDO	O1-C1-C2-O2
4	А	1206	EDO	O1-C1-C2-O2
3	А	1203	VVP	C9-C2-O1-C1

There are no ring outliers.

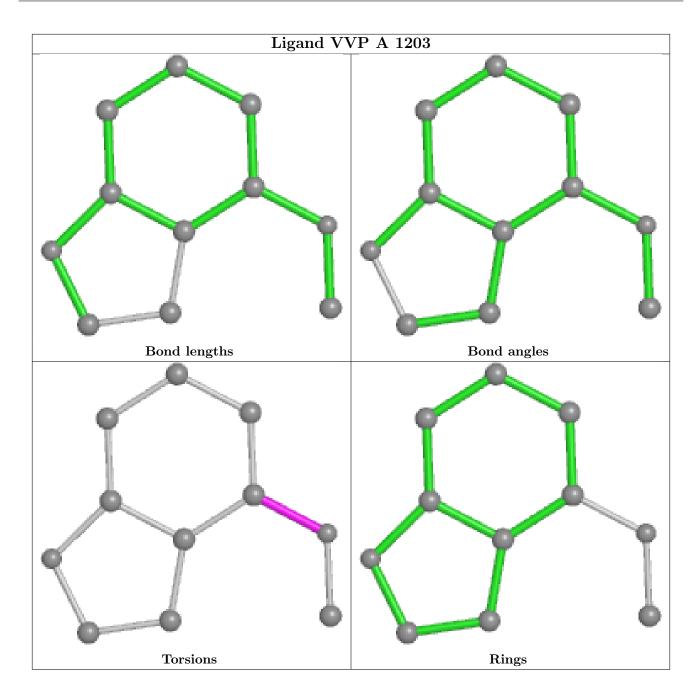
No monomer is involved in short contacts.

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	1104/1142~(96%)	-0.15	18 (1%)	72	70	12, 25, 54, 80	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	338	VAL	3.8
1	А	46	ALA	3.0
1	А	1112	LEU	3.0
1	А	748	GLY	2.7
1	А	1022	THR	2.7
1	А	342	GLU	2.5
1	А	768	SER	2.4
1	А	981	SER	2.4
1	А	548	ASP	2.4
1	А	94	SER	2.4
1	А	841	ALA	2.3
1	А	1109	VAL	2.2
1	А	243	ASP	2.2
1	А	687	TYR	2.2
1	А	71	GLY	2.2
1	А	767	SER	2.2
1	А	1111	ASN	2.1
1	А	418	ASN	2.1

## 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.

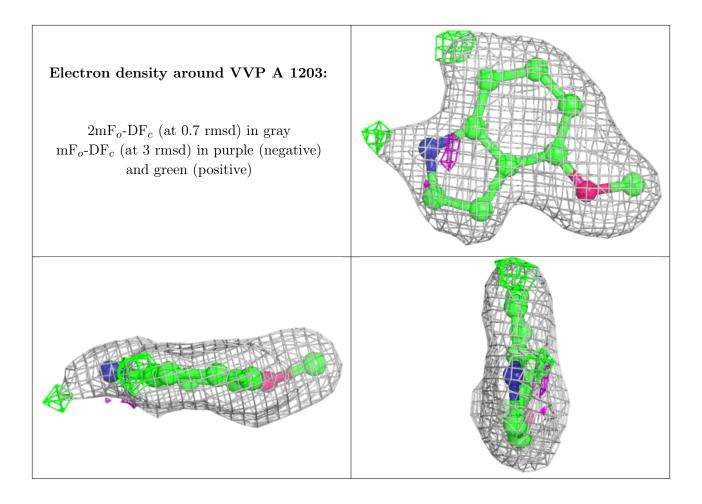
### 6.4 Ligands (i)

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.

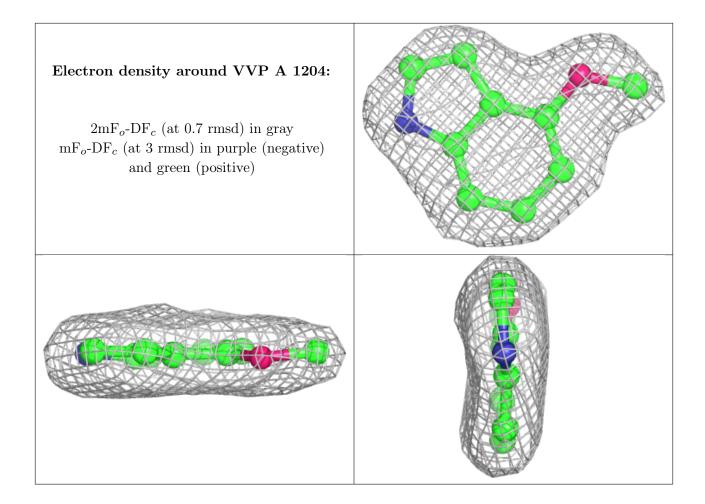
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	UNX	А	1210	1/1	0.70	0.27	33,33,33,33	0
5	UNX	А	1207	1/1	0.82	0.58	23,23,23,23	0
5	UNX	А	1208	1/1	0.86	0.45	$25,\!25,\!25,\!25$	0
3	VVP	А	1203	11/11	0.89	0.14	24,29,37,37	0
2	TLA	А	1202	10/10	0.89	0.20	$36,\!45,\!48,\!49$	0
5	UNX	А	1211	1/1	0.89	0.17	29,29,29,29	0
4	EDO	А	1205	4/4	0.91	0.23	16,19,24,31	0
5	UNX	А	1209	1/1	0.91	0.22	14,14,14,14	0
4	EDO	А	1206	4/4	0.93	0.17	23,26,26,34	0
3	VVP	А	1204	11/11	0.97	0.13	28,30,33,34	0
2	TLA	А	1201	10/10	0.97	0.12	21,27,33,38	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.

