



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 26, 2016 – 09:59 PM EDT

PDB ID : 5B5B  
Title : Crystal structure of VDR-LBD complexed with 2-methylidene-26,27-diphenyl  
-19-nor-1,25-dihydroxyvitamin D3  
Authors : Kato, A.; Itoh, T.; Yamamoto, K.  
Deposited on : 2016-05-02  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

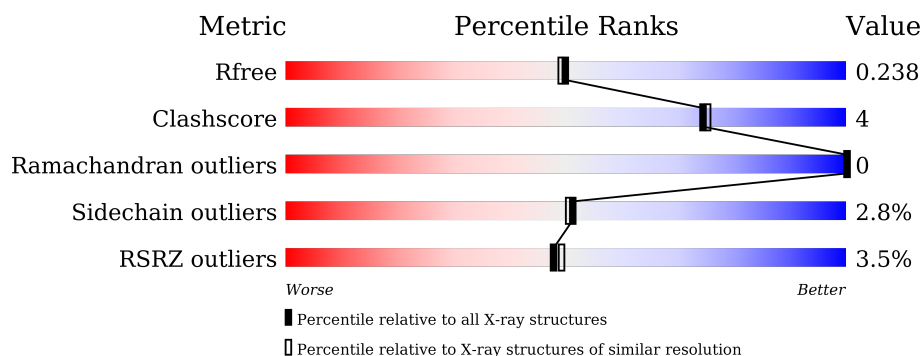
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	271	<div> <div>3%</div> <div>84% 8% 8%</div> </div>
1	D	271	<div> <div>2%</div> <div>79% 8% 11%</div> </div>
2	C	13	<div> <div>15%</div> <div>62% 15% 8% 15%</div> </div>
2	F	13	<div> <div>15%</div> <div>54% 31% 15%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4470 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 Vitamin D3 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1986	1261	340	373	12			
1	D	240	Total	C	N	O	S	0	0	0
			1916	1217	327	360	12			

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	GLY	-	expression tag	UNP P13053
A	107	SER	-	expression tag	UNP P13053
A	108	HIS	-	expression tag	UNP P13053
A	109	MET	-	expression tag	UNP P13053
A	110	GLY	-	expression tag	UNP P13053
A	111	SER	-	expression tag	UNP P13053
A	112	PRO	-	expression tag	UNP P13053
A	113	ASN	-	expression tag	UNP P13053
A	114	SER	-	expression tag	UNP P13053
A	115	PRO	-	expression tag	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	TYR	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	PRO	deletion	UNP P13053
A	?	-	ARG	deletion	UNP P13053
A	?	-	PRO	deletion	UNP P13053
A	?	-	THR	deletion	UNP P13053
A	?	-	LEU	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	PHE	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	GLY	deletion	UNP P13053
A	?	-	ASN	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	ASP	deletion	UNP P13053
A	?	-	LEU	deletion	UNP P13053
A	?	-	TYR	deletion	UNP P13053
A	?	-	THR	deletion	UNP P13053
A	?	-	THR	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	LEU	deletion	UNP P13053
A	?	-	ASP	deletion	UNP P13053
A	?	-	MET	deletion	UNP P13053
A	?	-	MET	deletion	UNP P13053
A	?	-	GLU	deletion	UNP P13053
A	?	-	PRO	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	GLY	deletion	UNP P13053
A	?	-	PHE	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	ASN	deletion	UNP P13053
A	?	-	LEU	deletion	UNP P13053
A	?	-	ASP	deletion	UNP P13053
A	?	-	LEU	deletion	UNP P13053
A	?	-	ASN	deletion	UNP P13053
A	?	-	GLY	deletion	UNP P13053
A	?	-	GLU	deletion	UNP P13053
A	?	-	ASP	deletion	UNP P13053
A	?	-	SER	deletion	UNP P13053
A	?	-	ASP	deletion	UNP P13053
A	?	-	ASP	deletion	UNP P13053
A	?	-	PRO	deletion	UNP P13053
D	106	GLY	-	expression tag	UNP P13053
D	107	SER	-	expression tag	UNP P13053
D	108	HIS	-	expression tag	UNP P13053
D	109	MET	-	expression tag	UNP P13053
D	110	GLY	-	expression tag	UNP P13053
D	111	SER	-	expression tag	UNP P13053
D	112	PRO	-	expression tag	UNP P13053
D	113	ASN	-	expression tag	UNP P13053
D	114	SER	-	expression tag	UNP P13053
D	115	PRO	-	expression tag	UNP P13053

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	SER	deletion	UNP P13053
D	?	-	TYR	deletion	UNP P13053
D	?	-	SER	deletion	UNP P13053
D	?	-	PRO	deletion	UNP P13053
D	?	-	ARG	deletion	UNP P13053
D	?	-	PRO	deletion	UNP P13053
D	?	-	THR	deletion	UNP P13053
D	?	-	LEU	deletion	UNP P13053
D	?	-	SER	deletion	UNP P13053
D	?	-	PHE	deletion	UNP P13053
D	?	-	SER	deletion	UNP P13053
D	?	-	GLY	deletion	UNP P13053
D	?	-	ASN	deletion	UNP P13053
D	?	-	SER	deletion	UNP P13053
D	?	-	SER	deletion	UNP P13053
D	?	-	SER	deletion	UNP P13053
D	?	-	SER	deletion	UNP P13053
D	?	-	SER	deletion	UNP P13053
D	?	-	ASP	deletion	UNP P13053
D	?	-	LEU	deletion	UNP P13053
D	?	-	TYR	deletion	UNP P13053
D	?	-	THR	deletion	UNP P13053
D	?	-	THR	deletion	UNP P13053
D	?	-	SER	deletion	UNP P13053
D	?	-	LEU	deletion	UNP P13053
D	?	-	ASP	deletion	UNP P13053
D	?	-	MET	deletion	UNP P13053
D	?	-	MET	deletion	UNP P13053
D	?	-	GLU	deletion	UNP P13053
D	?	-	PRO	deletion	UNP P13053
D	?	-	SER	deletion	UNP P13053
D	?	-	GLY	deletion	UNP P13053
D	?	-	PHE	deletion	UNP P13053
D	?	-	SER	deletion	UNP P13053
D	?	-	ASN	deletion	UNP P13053
D	?	-	LEU	deletion	UNP P13053
D	?	-	ASP	deletion	UNP P13053
D	?	-	LEU	deletion	UNP P13053
D	?	-	ASN	deletion	UNP P13053
D	?	-	GLY	deletion	UNP P13053
D	?	-	GLU	deletion	UNP P13053

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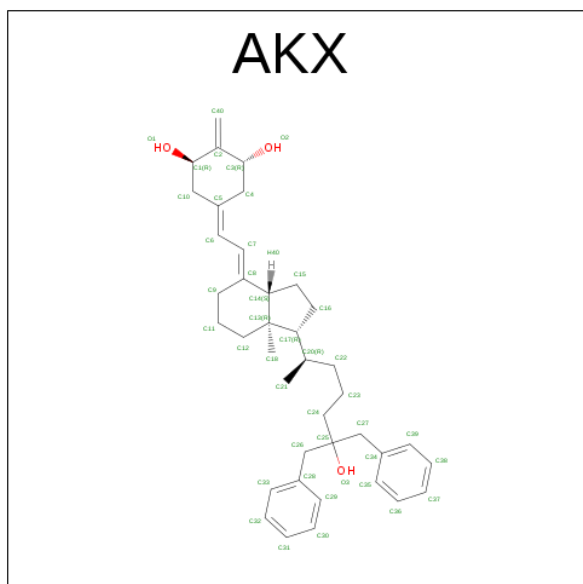
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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ASP	deletion	UNP P13053
D	?	-	SER	deletion	UNP P13053
D	?	-	ASP	deletion	UNP P13053
D	?	-	ASP	deletion	UNP P13053
D	?	-	PRO	deletion	UNP P13053

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	S	0	0	0
			91	59	17	13	2			
2	F	11	Total	C	N	O	S	0	0	0
			87	56	16	13	2			

- Molecule 3 is (1R,3R)-5-[(2E)-2-[(1R,3aS,7aR)-7a-methyl-1-[(2R)-6-oxidanyl-7-phenyl-6-(phenylmethyl)heptan-2-yl]-2,3,3a,5,6,7-hexahydro-1H-inden-4-ylidene]ethylidene]-2-methylidene-cyclohexane-1,3-diol (three-letter code: AKX) (formula: C<sub>39</sub>H<sub>52</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			42	39	3		
3	D	1	Total	C	O	0	0
			42	39	3		

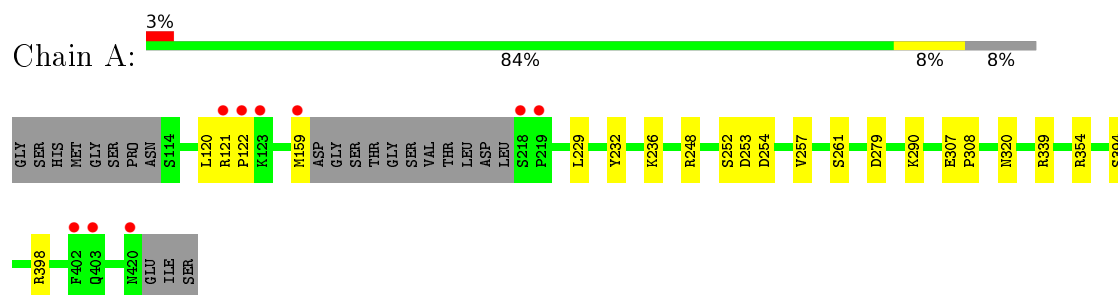
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	162	Total 162	O 162	0	0
4	C	2	Total 2	O 2	0	0
4	D	140	Total 140	O 140	0	0
4	F	2	Total 2	O 2	0	0

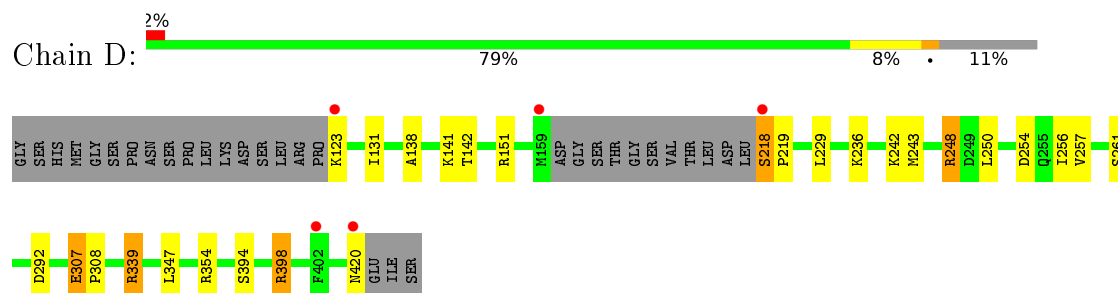
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

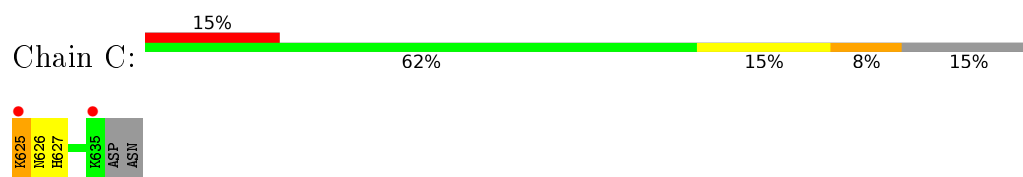
- Molecule 1: Vitamin D3 receptor



- Molecule 1: Vitamin D3 receptor



- Molecule 2: Mediator of RNA polymerase II transcription subunit 1



- Molecule 2: Mediator of RNA polymerase II transcription subunit 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.06 Å 41.49 Å 83.89 Å 90.00° 97.44° 90.00°	Depositor
Resolution (Å)	30.14 – 2.00 30.14 – 2.00	Depositor EDS
% Data completeness (in resolution range)	86.0 (30.14-2.00) 86.0 (30.14-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 2.00 Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.180 , 0.230 0.189 , 0.238	Depositor DCC
$R_{free}$ test set	1529 reflections (5.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.7	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 51.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4470	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.19 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.5820e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<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.

## 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: AKX

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	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.76	0/2028	0.81	0/2746
1	D	0.69	0/1956	0.76	0/2648
2	C	0.62	0/92	0.74	0/121
2	F	0.59	0/88	0.68	0/117
All	All	0.72	0/4164	0.78	0/5632

There are no bond length outliers.

There are no bond angle outliers.

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	1986	0	1990	13	0
1	D	1916	0	1914	19	1
2	C	91	0	102	1	0
2	F	87	0	91	2	1
3	A	42	0	0	0	0
3	D	42	0	0	0	0
4	A	162	0	0	1	0
4	C	2	0	0	0	0
4	D	140	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	2	0	0	0	0
All	All	4470	0	4097	33	1

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 4.

The worst 5 of 33 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:D:394:SER:O	1:D:398:ARG:HD3	1.74	0.88
1:A:394:SER:O	1:A:398:ARG:HG3	1.94	0.68
1:D:256:ILE:HG23	2:F:630:LEU:HD23	1.78	0.65
1:A:120:LEU:O	1:A:122:PRO:HD3	2.00	0.62
1:A:261:SER:OG	1:A:339:ARG:HD2	2.02	0.59

All (1) 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:151:ARG:NH1	2:F:626:ASN:OD1[1_565]	2.11	0.09

## 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	A	245/271 (90%)	242 (99%)	3 (1%)	0	100	100
1	D	236/271 (87%)	231 (98%)	5 (2%)	0	100	100
2	C	9/13 (69%)	9 (100%)	0	0	100	100
2	F	9/13 (69%)	8 (89%)	1 (11%)	0	100	100
All	All	499/568 (88%)	490 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	227/247 (92%)	223 (98%)	4 (2%)	66	69
1	D	218/247 (88%)	212 (97%)	6 (3%)	51	50
2	C	11/13 (85%)	9 (82%)	2 (18%)	2	1
2	F	10/13 (77%)	9 (90%)	1 (10%)	9	5
All	All	466/520 (90%)	453 (97%)	13 (3%)	51	50

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	626	ASN
1	D	218	SER
1	D	398	ARG
2	C	625	LYS
1	D	339	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	373	HIS
1	D	381	GLN
1	D	273	GLN
1	A	320	ASN
1	A	374	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	AKX	A	501	-	41,46,46	1.00	3 (7%)	51,66,66	1.53	8 (15%)
3	AKX	D	501	-	41,46,46	0.81	1 (2%)	51,66,66	1.28	7 (13%)

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	AKX	A	501	-	-	0/26/70/70	0/5/5/5
3	AKX	D	501	-	-	0/26/70/70	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	AKX	C13-C14	-2.04	1.52	1.56
3	A	501	AKX	C22-C20	-2.00	1.49	1.54
3	A	501	AKX	C26-C28	2.05	1.54	1.51
3	A	501	AKX	C7-C6	2.15	1.49	1.42

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	A	501	AKX	C6-C7-C8	-4.07	120.72	125.82
3	D	501	AKX	C6-C7-C8	-3.70	121.19	125.82
3	D	501	AKX	C16-C15-C14	-3.10	100.40	105.45
3	A	501	AKX	C16-C15-C14	-2.61	101.19	105.45
3	D	501	AKX	O1-C1-C2	-2.54	104.69	110.74

There are no chirality outliers.

There are no torsion outliers.

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](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	249/271 (91%)	-0.22	9 (3%) 46 48	10, 19, 40, 73	0
1	D	240/271 (88%)	-0.18	5 (2%) 67 67	12, 23, 45, 72	0
2	C	11/13 (84%)	0.46	2 (18%) 2 2	27, 30, 63, 67	0
2	F	11/13 (84%)	0.82	2 (18%) 2 2	30, 35, 74, 75	0
All	All	511/568 (89%)	-0.17	18 (3%) 48 49	10, 21, 45, 75	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	MET	7.1
1	A	402	PHE	6.8
1	D	402	PHE	6.5
1	D	159	MET	6.3
1	D	420	ASN	5.3

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	AKX	A	501	42/42	0.96	0.14	0.78	10,18,23,27	0
3	AKX	D	501	42/42	0.93	0.13	0.45	13,21,24,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.