



# Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2020 – 11:30 pm BST

PDB ID : 4UV9  
Title : LSD1(KDM1A)-CoREST in complex with 1-Ethyl-Tranylcypromine  
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Deposited on : 2014-08-05  
Resolution : 3.00 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](mailto: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 ⓘ 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

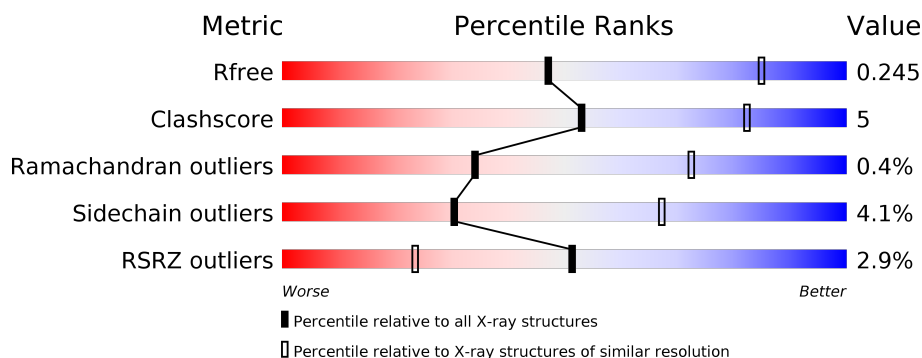
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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  $\leq 5\%$ . 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	872	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 24%, yellow 24%, yellow 64%, green 64%, green 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0;">64% 12% • 24%</div> </div> </div>
2	B	482	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">2%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 2%, orange 2%, orange 24%, yellow 24%, yellow 72%, green 72%, green 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0;">24% • 72%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6358 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 LYSINE-SPECIFIC HISTONE DEMETHYLASE 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	666	5217	3324	906	967	20	0	0	0

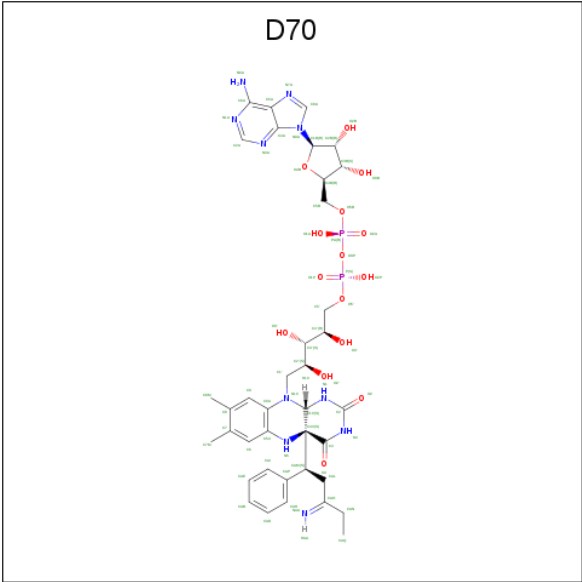
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	PRO	ALA	conflict	UNP O60341
A	?	-	ASP	deletion	UNP O60341
A	?	-	THR	deletion	UNP O60341
A	?	-	VAL	deletion	UNP O60341
A	?	-	LYS	deletion	UNP O60341

- Molecule 2 is a protein called REST COREPRESSOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	133	1076	676	194	203	3	0	0	0

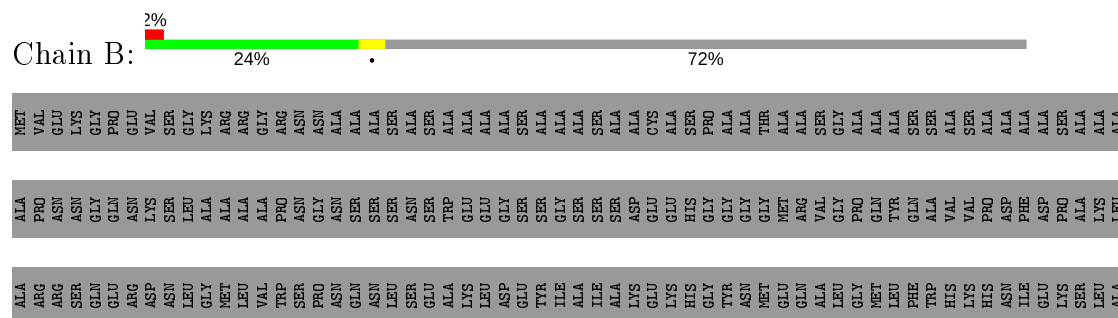
- Molecule 3 is [(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methyl (2R,3S,4S)-2,3,4-trihydroxy-5-[(4aS,10aS)-4a-[(1S,3E)-3-imino-1-phenylpentyl]-7,8-dimethyl-2,4-dioxo-1,3,4,4a,5,10a-hexahydrobenzo[g]pteridin-10(2H)-yl]pentyl dihydrogen diphosphate (three-letter code: D70) (formula: C<sub>38</sub>H<sub>50</sub>N<sub>10</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	65	38	10	15	2	0	0



- Molecule 1: LYSINE-SPECIFIC HISTONE DEMETHYLASE 1A



GLU	GLN	ASP	SER
ALA	ALA	LEU	LEU
LYS	LYS	PRO	PRO
ASN	ASN	ASN	ASN
GLY	ARG	PHE	THR
PRO	ALA	HIS	THR
SER	LYS	PRO	PRO
ASN	R308	ARG	PHE
GLN	R309	LYS	PRO
LYS	F310	GLN	ASP
PRO	F311	LYS	GLU
VAL	R312	ARG	TRP
LYS	G313	GLU	THR
SER	R314	ARG	VAL
PRO	F315	GLU	GLU
ASP	I316	GLU	ASP
ASN	S317	SER	LYS
SER		GLU	VAL
ILE	V321	ASP	LEU
LYS		GLU	PHE
MET	T332	LEU	GLU
PRO		GLU	GLN
GLU	Q337	GLU	ALA
GLU		ALA	PHE
GLU	R347	ASN	SER
ASP	G348	GLY	PHE
GLU	I349	ASN	HIS
ALA		ASN	GLY
PRO	N356	PRO	LYS
VAL		ILE	THR
LEU	I363	ASP	PHE
ASP	R364	ILE	HIS
VAL	G365	GLU	ARG
ARG	G366	VAL	ILE
TYR	T367	ASP	GLN
ALA	E368	GLN	GLN
SER	P369	ASN	MET
ALA	Y370	LYS	LEU
SER		GLU	PRO
	F373	SER	ASP
	E374	LYS	LYS
	V375	LYS	SER
	I376	GLU	ILE
		VAL	ALA
	G399	PRO	SER
		PRO	LEU
	A404	THR	VAL
		GLU	LYS
	D407	THR	PHE
		VAL	TYR
	V417	PRO	TYR
		GLN	SER
	F421	VAL	TRP
		LYS	LYS
	I434	LYS	LYS
		GLU	THR
	E440	LYS	ARG
	HIS	HIS	THR
	GLY	SER	LYS
	LYS	THR	THR

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.30Å 178.56Å 234.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.23 – 3.00 53.17 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (53.23-3.00) 99.3 (53.17-3.00)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.7.0027	Depositor
R, $R_{free}$	0.226 , 0.246 0.228 , 0.245	Depositor DCC
$R_{free}$ test set	971 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.7	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6358	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: D70

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	0.43	3/5331 (0.1%)	0.51	1/7232 (0.0%)
2	B	0.39	0/1091	0.47	0/1471
All	All	0.42	3/6422 (0.0%)	0.50	1/8703 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	531	TRP	CD2-CE2	5.23	1.47	1.41
1	A	646	TRP	CD2-CE2	5.19	1.47	1.41
1	A	431	TRP	CD2-CE2	5.03	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	815	LEU	CA-CB-CG	5.16	127.17	115.30

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	5217	0	5252	65	0
2	B	1076	0	1091	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	65	0	46	3	0
All	All	6358	0	6389	69	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 5.

All (69) 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:384:ARG:HB3	2:B:314:MET:HE1	1.43	0.99
1:A:533:PHE:O	1:A:537:GLU:HG3	1.88	0.73
1:A:435:VAL:HG13	2:B:349:ILE:HG13	1.71	0.73
1:A:548:SER:O	1:A:552:TRP:HB3	1.96	0.63
1:A:801:GLU:HG2	1:A:809:ALA:H	1.65	0.62
1:A:384:ARG:HB3	2:B:314:MET:CE	2.27	0.59
1:A:485:ARG:HG3	2:B:407:ASP:HB2	1.85	0.59
1:A:463:LYS:O	1:A:467:GLU:HG2	2.04	0.58
1:A:566:THR:HG21	1:A:697:LEU:HD13	1.85	0.58
1:A:331:ALA:HB2	3:A:900:D70:H10	1.86	0.57
1:A:331:ALA:CB	3:A:900:D70:H10	2.37	0.55
1:A:793:ILE:H	1:A:793:ILE:HD12	1.72	0.55
1:A:801:GLU:HG2	1:A:809:ALA:N	2.21	0.55
1:A:601:GLU:HA	1:A:616:TYR:O	2.09	0.53
1:A:342:MET:HG2	1:A:812:HIS:HB3	1.91	0.52
1:A:755:PRO:HA	1:A:758:ARG:NH1	2.23	0.52
1:A:801:GLU:CG	1:A:809:ALA:HA	2.39	0.52
1:A:353:LEU:HB3	1:A:565:LEU:HD22	1.92	0.52
1:A:720:ASP:O	1:A:724:VAL:HG23	2.09	0.52
1:A:364:GLU:HA	1:A:681:VAL:HB	1.93	0.51
1:A:537:GLU:HG2	1:A:544:LEU:HG	1.93	0.51
1:A:693:LEU:HD12	1:A:694:PHE:H	1.76	0.51
1:A:661:LYS:HB3	1:A:704:LEU:HD21	1.93	0.50
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.77	0.50
1:A:707:VAL:HG12	1:A:712:ALA:HA	1.94	0.49
1:A:487:LEU:HD21	2:B:370:TYR:O	2.11	0.49
1:A:695:TRP:CE3	1:A:697:LEU:HD11	2.47	0.48
1:A:772:ASP:HA	1:A:775:LEU:HD12	1.94	0.48
1:A:180:GLN:HA	1:A:339:GLY:HA2	1.94	0.48
1:A:592:GLN:HB3	1:A:603:ILE:HD12	1.94	0.48
1:A:677:LEU:HB2	1:A:693:LEU:HD11	1.95	0.48
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ILE:HG12	1:A:590:VAL:HG21	1.96	0.47
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.80	0.47
1:A:270:ILE:O	1:A:272:PRO:HD3	2.15	0.47
1:A:452:LYS:O	1:A:456:LYS:HB2	2.14	0.47
1:A:438:GLN:HB2	1:A:438:GLN:HE21	1.62	0.46
1:A:538:PHE:CZ	3:A:900:D70:HAE	2.51	0.46
1:A:485:ARG:HG3	2:B:407:ASP:CB	2.45	0.46
2:B:310:PRO:HB3	2:B:316:LEU:HD12	1.98	0.46
1:A:453:GLU:OE1	1:A:453:GLU:HA	2.16	0.45
1:A:428:ILE:O	1:A:432:LYS:HB2	2.17	0.45
1:A:541:ALA:O	1:A:657:GLY:HA3	2.17	0.45
1:A:356:ILE:HD11	1:A:566:THR:HG23	1.98	0.45
1:A:594:ARG:HG2	1:A:640:VAL:HB	1.98	0.45
1:A:535:ASN:HA	1:A:535:ASN:HD22	1.62	0.44
1:A:773:TYR:CE2	1:A:808:PRO:HB3	2.52	0.44
2:B:317:SER:O	2:B:321:VAL:HG23	2.18	0.44
2:B:417:VAL:O	2:B:421:PHE:HD1	2.01	0.43
1:A:454:LYS:O	1:A:458:LEU:HB2	2.18	0.43
1:A:435:VAL:O	1:A:439:GLU:HB2	2.20	0.42
1:A:392:LEU:HD23	1:A:398:PHE:CD2	2.55	0.42
1:A:473:ASP:OD1	1:A:473:ASP:C	2.57	0.42
1:A:801:GLU:HG3	1:A:809:ALA:HA	2.01	0.42
1:A:341:PRO:HG2	1:A:812:HIS:HB2	2.00	0.42
1:A:661:LYS:HD3	1:A:704:LEU:HD21	2.01	0.42
1:A:205:GLN:O	1:A:209:VAL:HG23	2.20	0.42
1:A:485:ARG:HD2	2:B:404:ALA:HA	2.01	0.42
1:A:188:MET:HG2	1:A:210:PHE:CE2	2.54	0.41
1:A:776:MET:HB3	1:A:803:THR:HG22	2.02	0.41
1:A:452:LYS:HE3	2:B:366:GLY:O	2.21	0.41
1:A:718:ILE:HG22	1:A:723:ILE:HG13	2.02	0.41
1:A:694:PHE:HA	1:A:704:LEU:O	2.20	0.41
1:A:656:PHE:HA	1:A:762:SER:HA	2.03	0.41
1:A:289:SER:HB3	1:A:814:ALA:HB1	2.02	0.40
1:A:292:ALA:HB2	1:A:815:LEU:HD22	2.03	0.40
1:A:199:ILE:HD11	1:A:248:LEU:CD1	2.50	0.40
1:A:521:LEU:HD22	1:A:525:ASP:HB3	2.04	0.40
2:B:376:ILE:H	2:B:376:ILE:HG13	1.76	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	664/872 (76%)	634 (96%)	27 (4%)	3 (0%)	29	68
2	B	131/482 (27%)	121 (92%)	10 (8%)	0	100	100
All	All	795/1354 (59%)	755 (95%)	37 (5%)	3 (0%)	34	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	ASN
1	A	608	ARG
1	A	468	VAL

### 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	566/711 (80%)	542 (96%)	24 (4%)	30	66
2	B	117/395 (30%)	113 (97%)	4 (3%)	37	72
All	All	683/1106 (62%)	655 (96%)	28 (4%)	30	67

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	206	THR
1	A	237	GLN

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Mol	Chain	Res	Type
1	A	247	VAL
1	A	429	GLU
1	A	435	VAL
1	A	438	GLN
1	A	449	VAL
1	A	458	LEU
1	A	469	LYS
1	A	492	LYS
1	A	514	ASN
1	A	535	ASN
1	A	538	PHE
1	A	563	SER
1	A	571	TYR
1	A	645	GLU
1	A	652	GLN
1	A	659	LEU
1	A	667	ASP
1	A	677	LEU
1	A	684	THR
1	A	704	LEU
1	A	706	LEU
2	B	332	THR
2	B	337	GLN
2	B	347	ARG
2	B	376	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	422	HIS
1	A	438	GLN
1	A	460	GLN
1	A	535	ASN
2	B	318	GLN
2	B	348	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	D70	A	900	-	61,71,71	1.80	10 (16%)	71,108,108	1.58	11 (15%)

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	D70	A	900	-	-	3/39/99/99	0/7/7/7

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	D70	C5X-C9A	7.86	1.49	1.40
3	A	900	D70	CAP-CAM	-6.98	1.41	1.51
3	A	900	D70	C8-C7	3.58	1.49	1.40
3	A	900	D70	CAQ-CAN	-2.65	1.39	1.51
3	A	900	D70	C5A-C4A	2.57	1.47	1.40
3	A	900	D70	C4X-N5	2.53	1.50	1.46
3	A	900	D70	CAO-NAA	2.44	1.33	1.27
3	A	900	D70	C4X-C4	-2.37	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	D70	C5X-N5	-2.26	1.35	1.38
3	A	900	D70	CAL-CAO	2.22	1.54	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	D70	C4X-C10-N10	7.13	116.75	109.36
3	A	900	D70	CAL-CAM-C4X	3.78	119.85	112.18
3	A	900	D70	N3-C2-N1	3.74	120.05	116.12
3	A	900	D70	CAL-CAM-CAP	-3.68	107.95	112.31
3	A	900	D70	N3A-C2A-N1A	-3.66	122.95	128.68
3	A	900	D70	C4-N3-C2	-3.20	121.20	126.04
3	A	900	D70	P-O3P-PA	-2.62	123.83	132.83
3	A	900	D70	C1B-N9A-C4A	-2.30	122.60	126.64
3	A	900	D70	C2A-N1A-C6A	2.24	122.59	118.75
3	A	900	D70	C4A-C5A-N7A	-2.07	107.24	109.40
3	A	900	D70	C5'-C4'-C3'	-2.03	108.28	112.20

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	900	D70	C4-C4X-CAM-CAL
3	A	900	D70	CAQ-CAN-CAO-CAL
3	A	900	D70	O4B-C4B-C5B-O5B

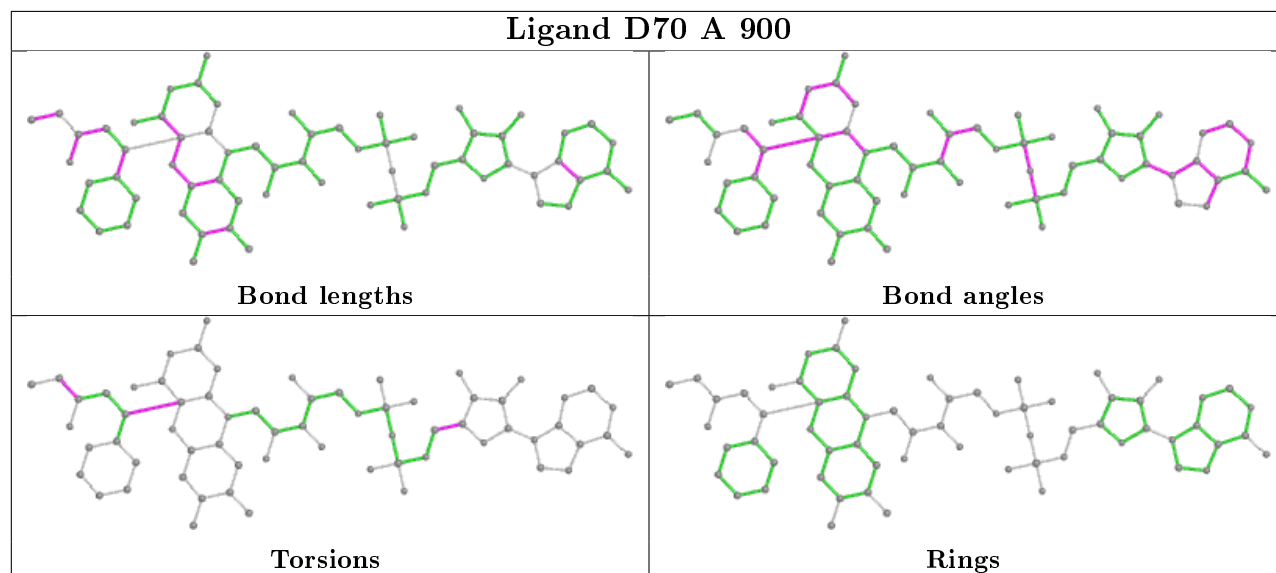
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	D70	3	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 than 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

### 6.1 Protein, DNA and RNA chains

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	666/872 (76%)	0.16	12 (1%) 68 40	36, 65, 104, 129	0
2	B	133/482 (27%)	0.65	11 (8%) 11 3	60, 95, 116, 144	0
All	All	799/1354 (59%)	0.24	23 (2%) 51 23	36, 71, 108, 144	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	374	GLU	4.8
2	B	376	ILE	3.5
1	A	500	THR	3.4
2	B	308	ARG	3.4
1	A	499	GLU	3.0
1	A	273	LEU	2.9
1	A	492	LYS	2.8
1	A	504	LEU	2.8
2	B	367	ILE	2.7
1	A	403	ASN	2.6
1	A	503	LYS	2.5
1	A	377	MET	2.4
1	A	436	LYS	2.3
2	B	369	PRO	2.3
2	B	365	GLY	2.2
2	B	312	LYS	2.1
1	A	447	LYS	2.1
2	B	373	PRO	2.1
2	B	434	LEU	2.1
1	A	174	VAL	2.1
2	B	399	GLY	2.0
1	A	242	TYR	2.0
2	B	363	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](#)

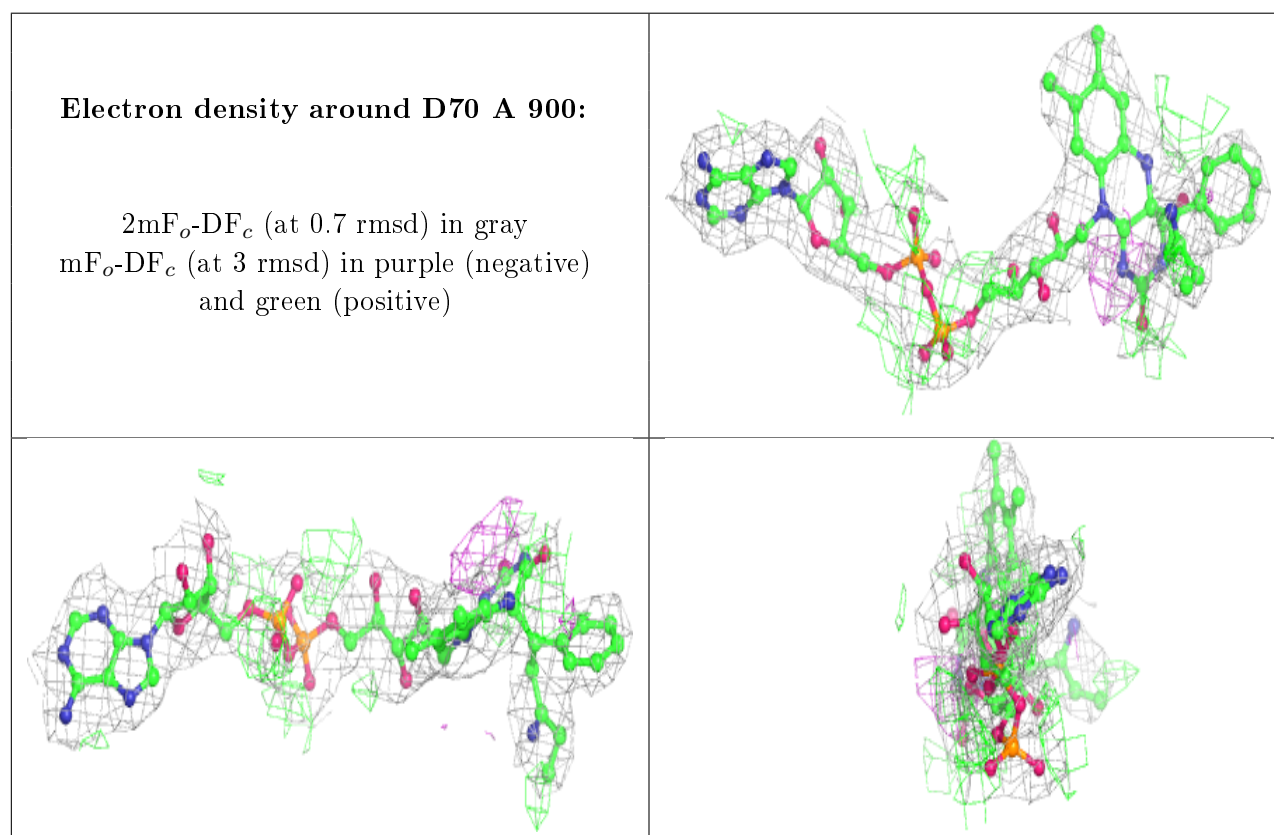
There are no carbohydrates in this entry.

## 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	D70	A	900	65/65	0.97	0.22	38,50,64,66	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.