



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 04:43 PM UTC

PDB ID : 4UVB / pdb_00004uvb
Title : LSD1(KDM1A)-CoREST in complex with 1-Methyl-Tranylcypromine (1S,2R)
Authors : Vianello, P.; Botrugno, O.; Cappa, A.; Ciossani, G.; Dessanti, P.; Mai, A.;
Mattevi, A.; Meroni, G.; Minucci, S.; Thaler, F.; Tortorici, M.; Trifiro, P.;
Valente, S.; Villa, M.; Varasi, M.; Mercurio, C.
Deposited on : 2014-08-05
Resolution : 2.80 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

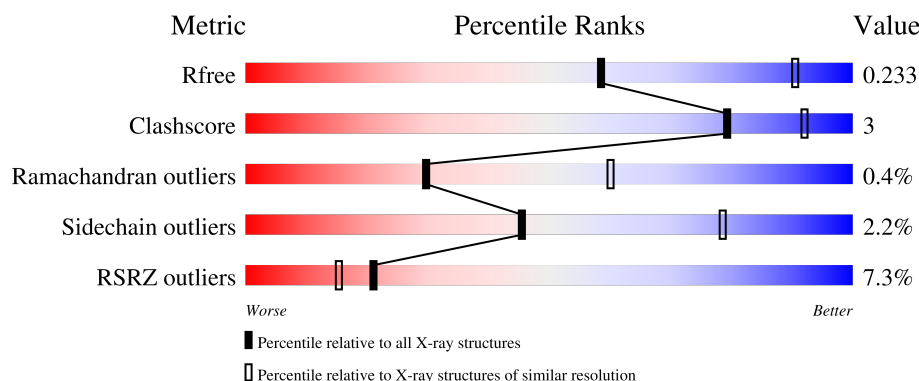
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. 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	
2	B	482	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	D51	A	900	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6356 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	5216	3323	906	967	20	0	0	0

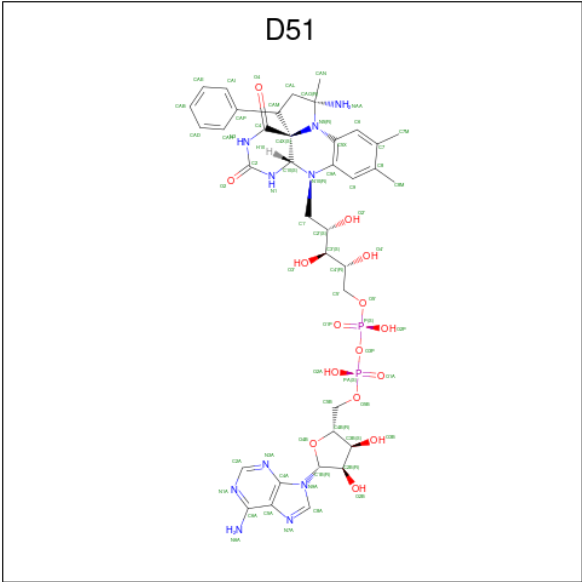
There are 5 discrepancies between the modelled and reference sequences:

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

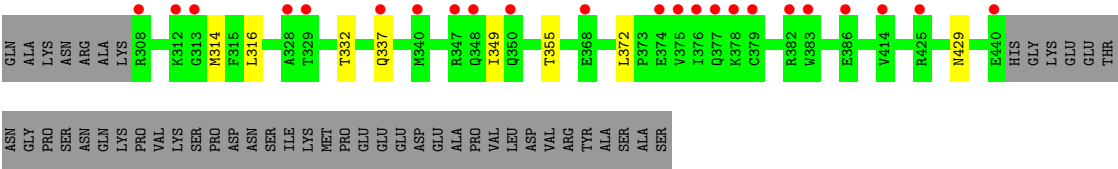
- Molecule 3 is [(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methyl (2R,3S,4S)-5-[(1R,3S,3aS,7aS)-1-amino-1,10,11-trimethyl-4,6-dioxo-3-phenyl-2,3,5,6,7,7a-hexahydro-1H-benzo[g]pyrrolo[2,1-e]pteridin-8(4H)-yl]-2,3,4-trihydroxypentyl dihydrogen diphosphate (CCD ID: D51) (formula: C₃₇H₄₈N₁₀O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	64	37	10	15	2	0	0

- Molecule 1: LYSINE-SPECIFIC HISTONE DEMETHYLASE 1A





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	119.16Å 180.04Å 234.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.80) 99.7 (50.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0027	Depositor
R, R_{free}	0.222 , 0.236 0.220 , 0.233	Depositor DCC
R_{free} test set	1195 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å ²)	78.0	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6356	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D51

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	0.55	1/5329 (0.0%)	0.76	0/7229
2	B	0.42	0/1091	0.78	0/1471
All	All	0.53	1/6420 (0.0%)	0.76	0/8700

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	331	ALA	CA-CB	5.62	1.62	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5216	0	5246	34	0
2	B	1076	0	1091	6	0
3	A	64	0	45	3	0
All	All	6356	0	6382	34	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 3.

All (34) 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:HE3	1.58	0.86
1:A:384:ARG:HB3	2:B:314:MET:CE	2.26	0.66
1:A:331:ALA:HB2	3:A:900:D51:H10	1.81	0.63
1:A:331:ALA:CB	3:A:900:D51:H10	2.30	0.60
1:A:548:SER:O	1:A:552:TRP:HB3	2.04	0.56
1:A:661:LYS:HD3	1:A:704:LEU:HD21	1.88	0.55
1:A:539:ALA:O	3:A:900:D51:HAE	2.09	0.53
1:A:484:HIS:CD2	2:B:372:LEU:HD13	2.44	0.53
1:A:374:LYS:HE3	1:A:525:ASP:OD1	2.09	0.53
1:A:695:TRP:CE3	1:A:697:LEU:HD11	2.45	0.52
1:A:463:LYS:O	1:A:467:GLU:HG2	2.10	0.52
1:A:801:GLU:HG2	1:A:809:ALA:H	1.75	0.52
1:A:364:GLU:HA	1:A:681:VAL:HB	1.94	0.50
1:A:435:VAL:HG13	2:B:349:ILE:HG13	1.95	0.49
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.93	0.49
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.95	0.48
1:A:501:GLN:O	1:A:505:GLU:HB2	2.13	0.47
1:A:353:LEU:HB3	1:A:565:LEU:HD22	1.97	0.47
1:A:435:VAL:CG1	2:B:349:ILE:HG13	2.46	0.45
1:A:662:VAL:HB	1:A:705:ALA:HB3	1.99	0.45
1:A:566:THR:HG21	1:A:697:LEU:HD13	1.99	0.45
1:A:435:VAL:O	1:A:439:GLU:HB2	2.16	0.44
1:A:695:TRP:HE3	1:A:697:LEU:HD21	1.83	0.44
1:A:180:GLN:HA	1:A:339:GLY:HA2	1.99	0.44
1:A:468:VAL:O	1:A:472:ARG:NH1	2.45	0.43
1:A:537:GLU:HG3	1:A:544:LEU:HG	2.01	0.42
1:A:801:GLU:CG	1:A:809:ALA:HA	2.49	0.42
1:A:594:ARG:HG2	1:A:640:VAL:HB	2.02	0.42
1:A:592:GLN:HB3	1:A:603:ILE:HD12	2.02	0.41
1:A:801:GLU:HG2	1:A:809:ALA:N	2.35	0.41
1:A:601:GLU:HA	1:A:616:TYR:O	2.20	0.41
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.55	0.41
1:A:428:ILE:O	1:A:432:LYS:HB2	2.20	0.41
1:A:537:GLU:CG	1:A:544:LEU:HG	2.52	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%)	646 (97%)	16 (2%)	2 (0%)	36	66
2	B	131/482 (27%)	128 (98%)	2 (2%)	1 (1%)	16	44
All	All	795/1354 (59%)	774 (97%)	18 (2%)	3 (0%)	30	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	429	ASN
1	A	801	GLU
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	565/711 (80%)	553 (98%)	12 (2%)	47	79
2	B	117/395 (30%)	114 (97%)	3 (3%)	40	75
All	All	682/1106 (62%)	667 (98%)	15 (2%)	45	78

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	392	LEU
1	A	429	GLU
1	A	438	GLN

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Mol	Chain	Res	Type
1	A	458	LEU
1	A	469	LYS
1	A	492	LYS
1	A	556	ASP
1	A	633	GLN
1	A	645	GLU
1	A	659	LEU
1	A	684	THR
1	A	704	LEU
2	B	316	LEU
2	B	332	THR
2	B	337	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	259	HIS
1	A	296	GLN
1	A	380	GLN
1	A	395	GLN
1	A	410	GLN
1	A	427	GLN
1	A	438	GLN
1	A	459	HIS
1	A	484	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 oligosaccharides in this entry.

5.6 Ligand geometry

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	D51	A	900	-	63,71,71	1.73	7 (11%)	81,112,112	1.59	14 (17%)

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	D51	A	900	-	1/1/17/19	4/38/109/109	0/8/8/8

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	D51	CAP-CAM	-7.97	1.39	1.51
3	A	900	D51	C9A-C5X	5.20	1.50	1.41
3	A	900	D51	C5A-C4A	4.79	1.47	1.39
3	A	900	D51	C8-C7	3.62	1.49	1.40
3	A	900	D51	C5A-C6A	2.90	1.49	1.41
3	A	900	D51	C8A-N7A	2.46	1.36	1.31
3	A	900	D51	P-O3P	2.14	1.61	1.59

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	D51	C5A-C4A-N3A	-5.41	119.27	126.72
3	A	900	D51	N3-C2-N1	4.42	120.50	116.06
3	A	900	D51	N3A-C4A-N9A	4.37	134.60	127.17
3	A	900	D51	N3A-C2A-N1A	-3.85	122.75	128.58
3	A	900	D51	C2A-N3A-C4A	3.81	121.13	111.83
3	A	900	D51	C4A-C5A-N7A	-3.38	106.72	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	D51	C4A-N9A-C8A	2.97	108.86	105.74
3	A	900	D51	C4-N3-C2	-2.86	121.77	126.04
3	A	900	D51	CAL-CAM-CAP	-2.53	110.42	115.94
3	A	900	D51	C5A-N7A-C8A	2.49	107.37	103.45
3	A	900	D51	C6A-C5A-N7A	2.46	136.83	132.09
3	A	900	D51	O4-C4-N3	-2.42	116.67	120.59
3	A	900	D51	C2A-N1A-C6A	2.22	122.38	118.73
3	A	900	D51	N9A-C8A-N7A	-2.13	110.92	113.94

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	900	D51	CAM

All (4) torsion outliers are listed below:

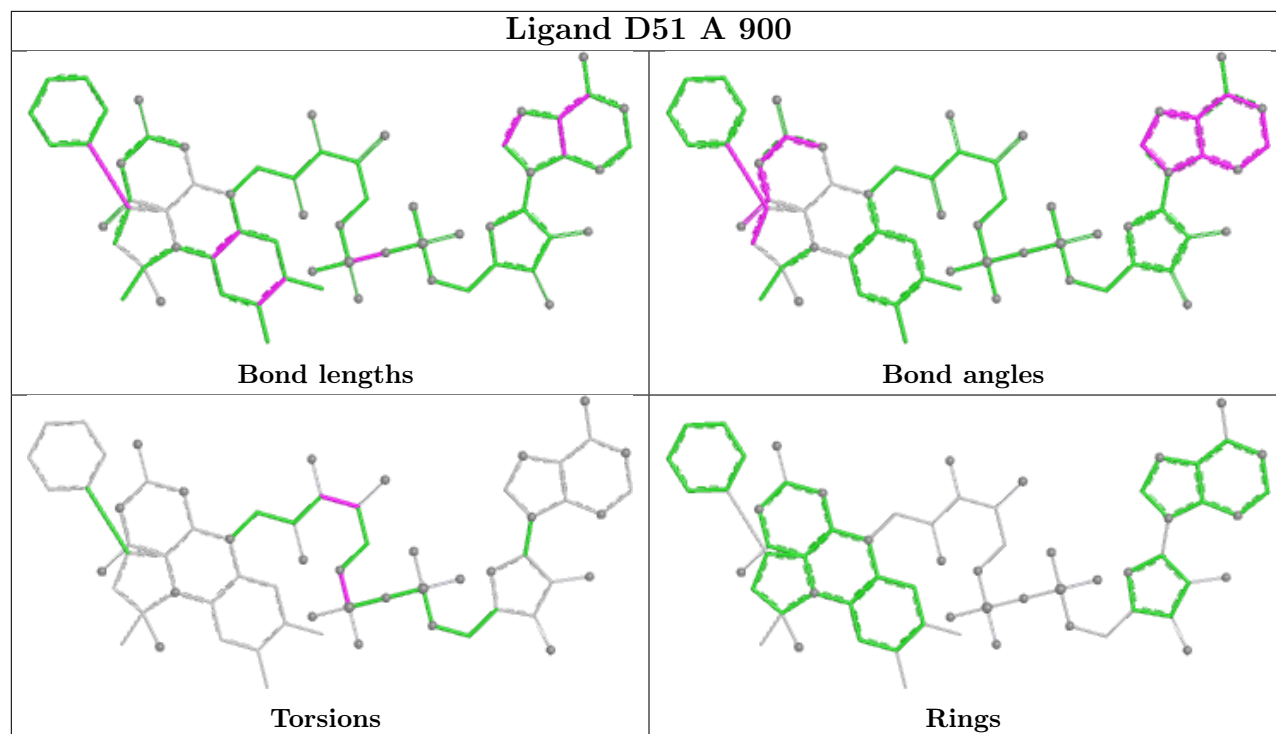
Mol	Chain	Res	Type	Atoms
3	A	900	D51	C2'-C3'-C4'-O4'
3	A	900	D51	C5'-O5'-P-O1P
3	A	900	D51	O3'-C3'-C4'-O4'
3	A	900	D51	O3'-C3'-C4'-C5'

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	D51	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, 95th 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	A	666/872 (76%)	0.37	35 (5%) 32 24	46, 76, 112, 146	0
2	B	133/482 (27%)	1.07	23 (17%) 4 3	70, 106, 129, 146	0
All	All	799/1354 (59%)	0.48	58 (7%) 21 15	46, 82, 120, 146	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	836	LEU	11.7
2	B	376	ILE	6.0
1	A	171	PRO	5.7
1	A	275	THR	4.9
1	A	833	MET	4.3
1	A	786	ILE	3.8
1	A	835	THR	3.8
1	A	377	MET	3.8
2	B	337	GLN	3.7
1	A	273	LEU	3.6
1	A	272	PRO	3.5
2	B	377	GLN	3.5
1	A	271	LYS	3.4
2	B	440	GLU	3.3
2	B	340	MET	3.2
1	A	834	TYR	3.1
2	B	374	GLU	3.0
1	A	269	ARG	3.0
2	B	313	GLY	3.0
1	A	172	SER	2.9
1	A	511	LEU	2.8
1	A	274	PRO	2.8
2	B	414	VAL	2.8
2	B	382	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	328	ALA	2.7
1	A	268	LYS	2.7
2	B	312	LYS	2.7
2	B	378	LYS	2.7
2	B	329	THR	2.6
2	B	348	GLN	2.6
1	A	684	THR	2.6
1	A	358	GLN	2.5
2	B	350	GLN	2.5
1	A	787	PRO	2.5
1	A	373	GLU	2.5
1	A	506	GLU	2.5
1	A	667	ASP	2.4
2	B	347	ARG	2.4
1	A	492	LYS	2.4
2	B	379	CYS	2.3
2	B	308	ARG	2.3
2	B	375	VAL	2.3
1	A	739	ALA	2.3
1	A	270	ILE	2.3
2	B	383	TRP	2.3
1	A	744	LYS	2.3
1	A	203	PRO	2.2
1	A	695	TRP	2.2
1	A	357	LYS	2.2
1	A	467	GLU	2.2
2	B	425	ARG	2.1
1	A	372	LYS	2.1
1	A	237	GLN	2.1
2	B	386	GLU	2.1
1	A	503	LYS	2.1
1	A	510	GLU	2.1
1	A	519	VAL	2.0
2	B	368	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

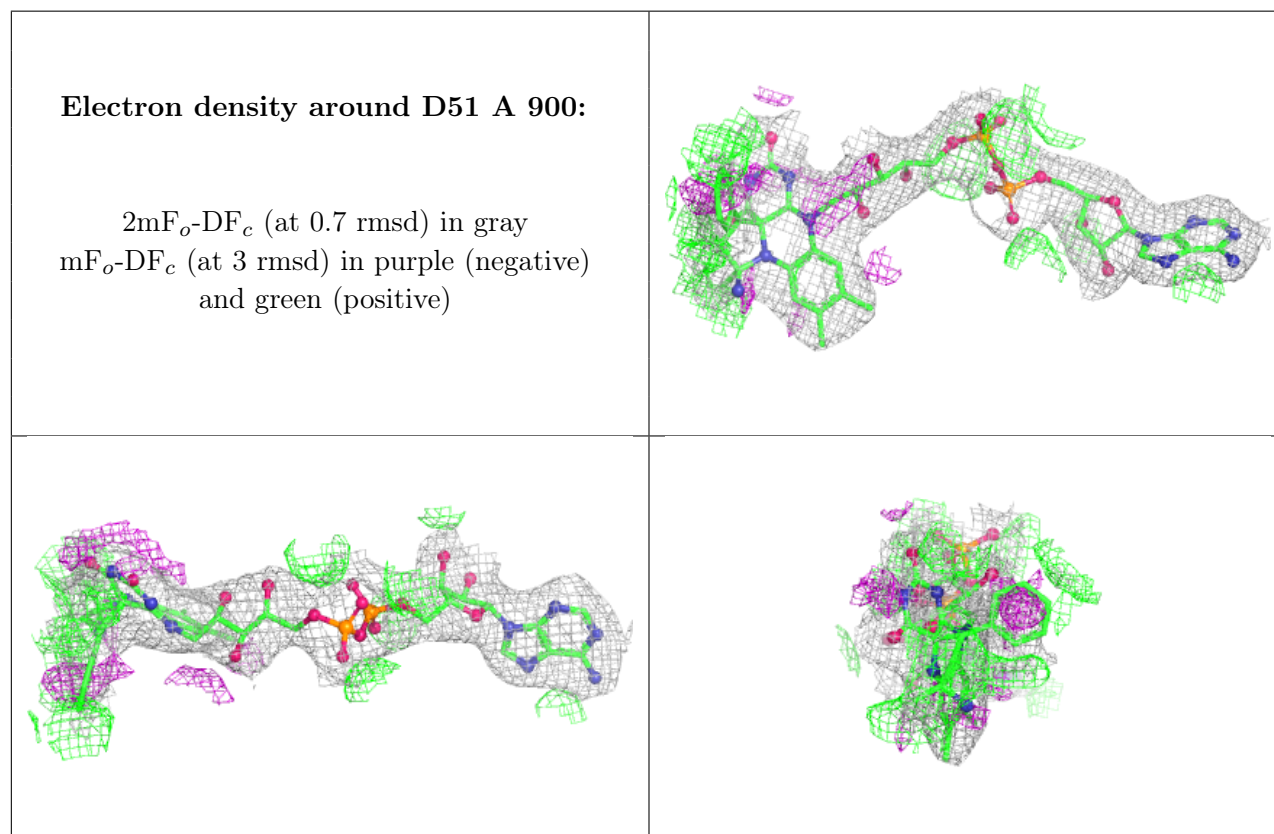
There are no oligosaccharides in this entry.

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, 95th 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	D51	A	900	64/64	0.95	0.11	49,61,102,107	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.