



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 08:28 am BST

PDB ID : 4UVC
Title : LSD1(KDM1A)-CoREST in complex with 1-Phenyl-Tranylcypromine
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 : 3.10 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 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

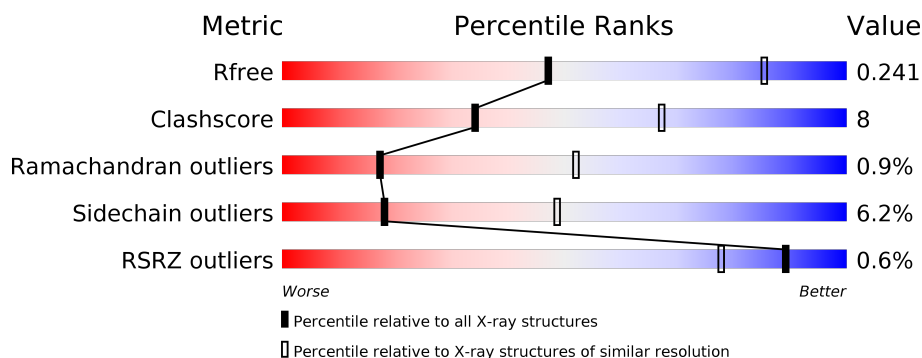
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 ≥ 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> <div></div> <div>59%</div> <div>16%</div> <div>24%</div> </div> </div>
2	B	482	<div> <div> <div>21%</div> <div>5%</div> <div>72%</div> </div> </div>

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	D52	A	900	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6361 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

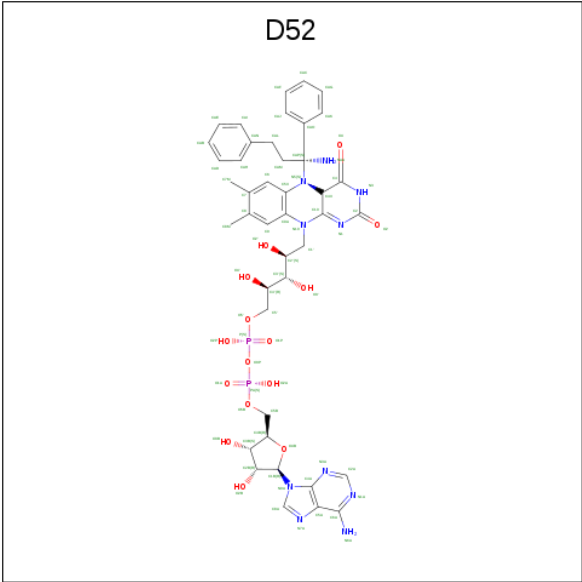
There are 5 discrepancies between the modelled and reference sequences:

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-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2R,3S,4S)-5-[5-[(1S)-1-azanyl-1,3-diphenyl-propyl]-7,8-dimethyl-2,4-bis(oxidanylidene)-4aH-benzo[g]pteridin-10-yl]-2,3,4-tris(oxidanyl)pentyl] hydrogen phosphate (three-letter code: D52) (formula: C₄₂H₅₀N₁₀O₁₅P₂).

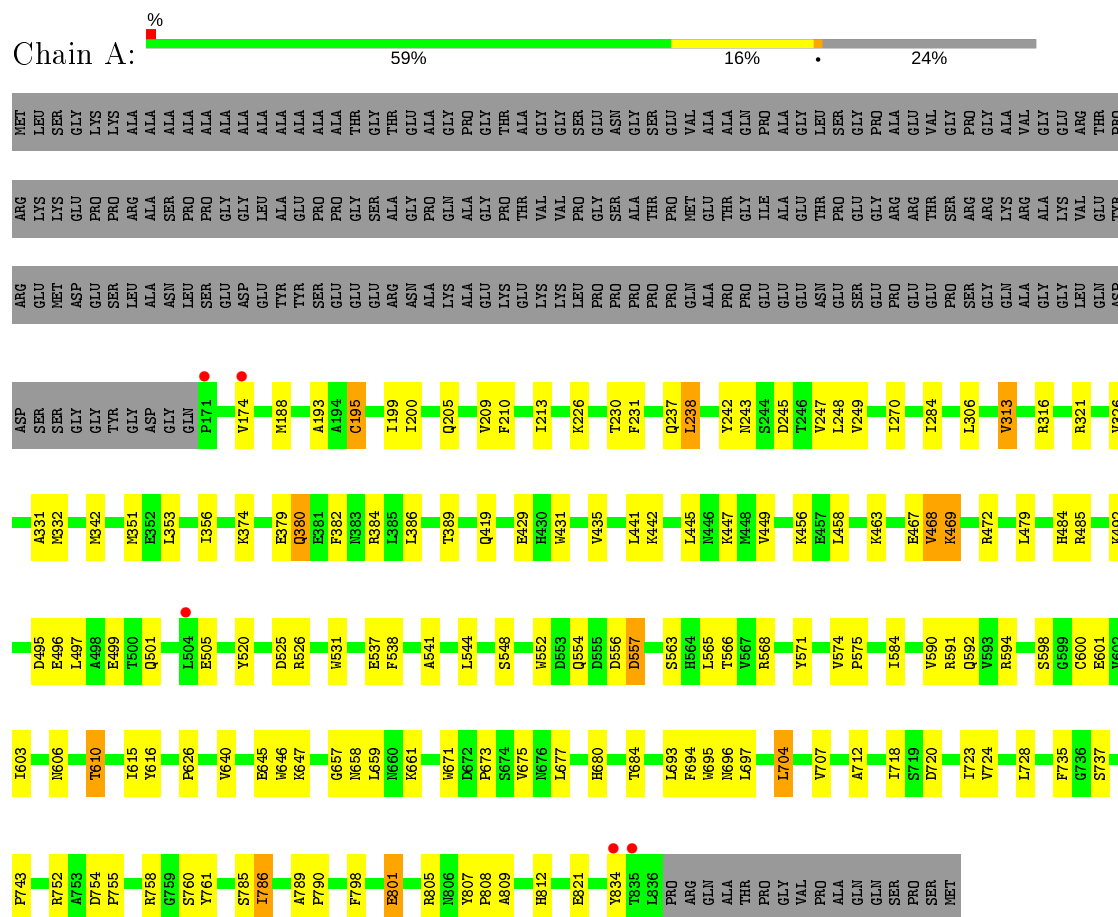


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			69	42	10	15	2		

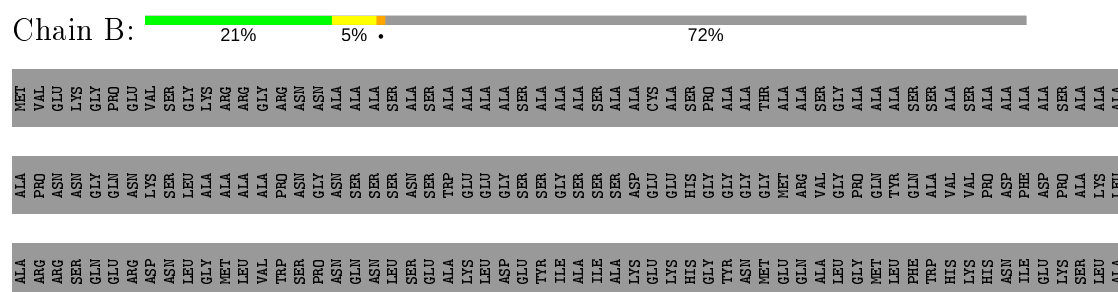
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: LYSINE-SPECIFIC HISTONE DEMETHYLASE 1A



• Molecule 2: REST COREPRESSOR 1



ASP	LEU	PRO	ASN	PHE	THR	PRO	PHE	PRO	PRO	ASN	ASP	GLU	TRP	THR	VAL	GLU	ASP	LYS	VAL	LEU	PHE	GLU	GLN	ALA	PHE	SER	PHE	HIS	GLY	LYS	THR	PHE	HIS	ARG	GLU	ASP	ILE	GLU	VAL	ASP	GLN	GLN	MET	LEU	PRO	ASP	LYS	SER	LYS	ILE	ALA	VAL	SER	LEU	VAL	THR	LYS	PHE	THR	TYR	TYR	GLN	TRP	LYS	LYS	THR	ARG	THR	LYS	SER	THR	THR																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
SER	VAL	MET	ASP	ARG	HIS	ALA	ARG	LYS	ARG	GLN	LYS	ARG	GLU	THR	ARG	GLU	GLU	SER	GLU	ASP	GLU	LEU	GLU	GLU	ALA	PHE	ASN	GLY	ASN	ASN	PRO	ILE	THR	ASP	ILE	GLU	ARG	VAL	ASP	GLN	GLN	ASN	MET	LYS	GLU	SER	SER	LYS	LYS	GLU	VAL	PRO	PRO	THR	VAL	GLU	THR	VAL	PRO	GLN	SER	VAL	LYS	LYS	GLU	LYS	ARG	THR	LYS	SER	THR	THR																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
GLN	ALA	LYS	ASN	ARG	ALA	LYS	R308	K312	G313	M314	F315	L316	S317	V321	V324	N327	A330	A331	Q337	V343	R347	Q348	I349	T355	N356	I367	Y370	R371	L372	P373	C379	A404	V417	F421	R425	N429	L434	W437	E440																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	118.96 Å 179.09 Å 234.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.53 – 3.10 65.38 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (68.53-3.10) 100.0 (65.38-3.10)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.13 Å)	Xtriage
Refinement program	REFMAC 5.7.0027	Depositor
R, R_{free}	0.210 , 0.241 0.212 , 0.241	Depositor DCC
R_{free} test set	886 reflections (1.93%)	wwPDB-VP
Wilson B-factor (Å ²)	78.0	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6361	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: D52

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	0.46	3/5329 (0.1%)	0.55	0/7229
2	B	0.40	1/1091 (0.1%)	0.52	0/1471
All	All	0.45	4/6420 (0.1%)	0.55	0/8700

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	437	TRP	CD2-CE2	5.20	1.47	1.41
1	A	531	TRP	CD2-CE2	5.17	1.47	1.41
1	A	646	TRP	CD2-CE2	5.07	1.47	1.41
1	A	431	TRP	CD2-CE2	5.04	1.47	1.41

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	5216	0	5246	94	0
2	B	1076	0	1091	22	0
3	A	69	0	47	7	0
All	All	6361	0	6384	107	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 8.

All (107) 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:199:ILE:HD11	1:A:248:LEU:HD11	1.50	0.93
1:A:356:ILE:HD11	1:A:566:THR:HG23	1.66	0.76
1:A:456:LYS:HA	2:B:370:TYR:CE2	2.26	0.69
1:A:693:LEU:HD12	1:A:694:PHE:H	1.59	0.66
1:A:374:LYS:HE3	1:A:525:ASP:OD1	1.95	0.66
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.77	0.66
1:A:231:PHE:HE1	1:A:249:VAL:HG12	1.64	0.63
1:A:548:SER:O	1:A:552:TRP:HB3	1.99	0.62
1:A:563:SER:O	1:A:565:LEU:HD12	1.99	0.62
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.65	0.61
1:A:188:MET:HG2	1:A:210:PHE:HE2	1.65	0.60
1:A:463:LYS:O	1:A:467:GLU:HG2	2.01	0.60
1:A:188:MET:HG2	1:A:210:PHE:CE2	2.38	0.59
1:A:284:ILE:HD13	1:A:590:VAL:HG11	1.85	0.58
1:A:601:GLU:HA	1:A:616:TYR:O	2.03	0.58
1:A:693:LEU:HD12	1:A:694:PHE:N	2.18	0.58
1:A:306:LEU:HD13	1:A:584:ILE:HG12	1.85	0.58
1:A:755:PRO:HA	1:A:758:ARG:CZ	2.33	0.58
1:A:231:PHE:CE1	1:A:249:VAL:HG12	2.41	0.56
1:A:707:VAL:HG12	1:A:712:ALA:HA	1.87	0.56
1:A:801:GLU:CG	1:A:809:ALA:HA	2.35	0.56
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.72	0.55
1:A:661:LYS:HD3	1:A:704:LEU:HD21	1.88	0.55
2:B:327:ASN:ND2	2:B:330:ALA:HB2	2.22	0.55
1:A:695:TRP:CE3	1:A:697:LEU:HD11	2.42	0.54
1:A:195:CYS:HG	1:A:834:TYR:HE2	1.55	0.54
1:A:801:GLU:HG2	1:A:809:ALA:H	1.71	0.53
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.44	0.53
1:A:238:LEU:HB3	1:A:243:ASN:HB3	1.91	0.53
1:A:419:GLN:HB3	1:A:520:TYR:CE1	2.44	0.53
1:A:435:VAL:HG13	2:B:349:ILE:HG13	1.89	0.53
2:B:367:ILE:HG13	2:B:371:ARG:HH12	1.74	0.53
1:A:537:GLU:CG	1:A:544:LEU:HG	2.39	0.52
1:A:484:HIS:CD2	2:B:372:LEU:HD13	2.45	0.52
1:A:807:TYR:N	1:A:808:PRO:HD3	2.24	0.52
1:A:342:MET:HG2	1:A:812:HIS:HB3	1.93	0.51
1:A:801:GLU:HG2	1:A:809:ALA:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:900:D52:HAK	3:A:900:D52:O4	2.10	0.50
2:B:421:PHE:O	2:B:425:ARG:HG3	2.11	0.50
1:A:755:PRO:HA	1:A:758:ARG:NH1	2.26	0.50
1:A:786:ILE:H	1:A:786:ILE:HD12	1.76	0.50
1:A:353:LEU:HB3	1:A:565:LEU:CD2	2.41	0.50
1:A:435:VAL:CG1	2:B:349:ILE:HG13	2.42	0.50
1:A:205:GLN:O	1:A:209:VAL:HG23	2.12	0.49
1:A:592:GLN:HB3	1:A:603:ILE:HD12	1.93	0.49
1:A:209:VAL:O	1:A:213:ILE:HG13	2.12	0.49
1:A:419:GLN:HE22	2:B:315:PHE:H	1.60	0.49
1:A:821:GLU:HA	1:A:821:GLU:OE1	2.12	0.49
1:A:379:GLU:O	1:A:382:PHE:HB3	2.13	0.48
1:A:603:ILE:HG12	1:A:615:ILE:HD13	1.94	0.48
2:B:317:SER:O	2:B:321:VAL:HG23	2.14	0.48
1:A:537:GLU:HG3	1:A:544:LEU:HG	1.96	0.47
1:A:245:ASP:OD1	1:A:247:VAL:HG22	2.14	0.47
1:A:761:TYR:HE2	3:A:900:D52:NAA	2.13	0.47
2:B:324:VAL:HG13	2:B:331:ALA:HA	1.96	0.47
1:A:557:ASP:OD1	1:A:557:ASP:N	2.45	0.47
1:A:671:TRP:HA	1:A:735:PHE:CE2	2.50	0.47
1:A:316:ARG:HD3	1:A:760:SER:O	2.15	0.47
1:A:469:LYS:HA	1:A:469:LYS:HE3	1.97	0.46
1:A:677:LEU:HB2	1:A:693:LEU:HD11	1.97	0.46
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.97	0.46
1:A:594:ARG:HA	1:A:640:VAL:O	2.15	0.46
1:A:384:ARG:HB3	2:B:314:MET:CE	2.46	0.45
1:A:374:LYS:CE	1:A:525:ASP:OD1	2.64	0.45
2:B:347:ARG:HG3	2:B:348:GLN:N	2.30	0.45
1:A:695:TRP:HE3	1:A:697:LEU:HD11	1.80	0.45
1:A:606:ASN:O	1:A:610:THR:HA	2.16	0.45
1:A:647:LYS:HE3	1:A:798:PHE:CE2	2.51	0.45
1:A:447:LYS:HD3	1:A:497:LEU:HD21	1.99	0.45
1:A:695:TRP:HE3	1:A:697:LEU:HD21	1.81	0.45
1:A:671:TRP:O	1:A:673:PRO:HD3	2.17	0.44
1:A:380:GLN:HB3	1:A:380:GLN:HE21	1.62	0.44
1:A:193:ALA:HB2	1:A:200:ILE:HD13	2.00	0.44
1:A:331:ALA:HA	3:A:900:D52:C4X	2.48	0.44
1:A:353:LEU:HB3	1:A:565:LEU:HD22	1.99	0.44
3:A:900:D52:C6	3:A:900:D52:NAA	2.73	0.44
2:B:324:VAL:HG12	2:B:324:VAL:O	2.18	0.43
1:A:468:VAL:O	1:A:472:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ALA:O	1:A:657:GLY:HA3	2.18	0.43
2:B:421:PHE:HE2	2:B:434:LEU:HD11	1.83	0.43
1:A:230:THR:HG23	1:A:270:ILE:HD12	2.00	0.43
1:A:728:LEU:HD21	1:A:743:PRO:HD3	2.01	0.43
1:A:384:ARG:HB3	2:B:314:MET:HE1	2.00	0.43
1:A:789:ALA:HB1	1:A:790:PRO:HD2	1.99	0.43
1:A:332:MET:HG2	3:A:900:D52:CAG	2.49	0.43
1:A:386:LEU:O	1:A:389:THR:OG1	2.29	0.43
1:A:720:ASP:O	1:A:724:VAL:HG23	2.18	0.43
1:A:626:PRO:HD3	3:A:900:D52:H5BA	2.00	0.43
1:A:707:VAL:CG1	1:A:712:ALA:HA	2.49	0.42
1:A:754:ASP:HA	1:A:755:PRO:HD2	1.74	0.42
1:A:485:ARG:HD2	2:B:404:ALA:HB1	2.02	0.42
1:A:495:ASP:OD1	2:B:371:ARG:NH2	2.53	0.42
1:A:441:LEU:O	1:A:445:LEU:HG	2.20	0.41
1:A:658:ASN:ND2	1:A:752:ARG:HB2	2.35	0.41
1:A:321:ARG:HG2	1:A:326:VAL:HG22	2.02	0.41
1:A:496:GLU:O	1:A:499:GLU:HB3	2.19	0.41
1:A:501:GLN:O	1:A:505:GLU:HB2	2.20	0.41
1:A:718:ILE:HG22	1:A:723:ILE:HG13	2.03	0.41
1:A:801:GLU:HG3	3:A:900:D52:O3'	2.19	0.41
2:B:372:LEU:HA	2:B:373:PRO:HD2	1.84	0.41
2:B:337:GLN:HA	2:B:337:GLN:HE21	1.86	0.41
2:B:417:VAL:O	2:B:421:PHE:HD1	2.04	0.41
1:A:755:PRO:HA	1:A:758:ARG:NH2	2.35	0.41
1:A:574:VAL:HB	1:A:575:PRO:CD	2.51	0.40
1:A:195:CYS:SG	1:A:834:TYR:HE2	2.43	0.40
1:A:332:MET:SD	1:A:661:LYS:NZ	2.94	0.40
1:A:566:THR:HG21	1:A:697:LEU:HD22	2.04	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%)	613 (92%)	45 (7%)	6 (1%)	17	52
2	B	131/482 (27%)	117 (89%)	13 (10%)	1 (1%)	19	54
All	All	795/1354 (59%)	730 (92%)	58 (7%)	7 (1%)	17	52

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	VAL
2	B	429	ASN
1	A	801	GLU
1	A	554	GLN
1	A	805	ARG
1	A	468	VAL
1	A	785	SER

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%)	532 (94%)	33 (6%)	20	51
2	B	117/395 (30%)	108 (92%)	9 (8%)	13	41
All	All	682/1106 (62%)	640 (94%)	42 (6%)	18	49

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	VAL
1	A	195	CYS
1	A	226	LYS
1	A	237	GLN
1	A	238	LEU
1	A	313	VAL
1	A	351	MET
1	A	380	GLN
1	A	429	GLU

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Mol	Chain	Res	Type
1	A	449	VAL
1	A	458	LEU
1	A	469	LYS
1	A	479	LEU
1	A	492	LYS
1	A	526	ARG
1	A	538	PHE
1	A	556	ASP
1	A	557	ASP
1	A	568	ARG
1	A	571	TYR
1	A	591	ARG
1	A	598	SER
1	A	600	CYS
1	A	610	THR
1	A	645	GLU
1	A	659	LEU
1	A	675	VAL
1	A	680	HIS
1	A	684	THR
1	A	696	ASN
1	A	704	LEU
1	A	737	SER
1	A	786	ILE
2	B	312	LYS
2	B	316	LEU
2	B	337	GLN
2	B	343	VAL
2	B	347	ARG
2	B	348	GLN
2	B	349	ILE
2	B	371	ARG
2	B	379	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	237	GLN
1	A	380	GLN
1	A	438	GLN
1	A	461	GLN

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Mol	Chain	Res	Type
1	A	484	HIS
1	A	633	GLN
1	A	791	GLN
2	B	337	GLN

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 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	D52	A	900	-	67,76,76	1.76	9 (13%)	78,115,115	1.10	7 (8%)

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	D52	A	900	-	1/1/16/17	4/39/100/100	0/7/8/8

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	D52	CAP-CAO	-7.49	1.42	1.52
3	A	900	D52	C9A-C5X	5.80	1.50	1.40
3	A	900	D52	C4X-C4	-4.45	1.48	1.52
3	A	900	D52	CAL-CAN	-4.35	1.39	1.51
3	A	900	D52	C8-C7	3.21	1.48	1.40
3	A	900	D52	C5A-C4A	2.91	1.48	1.40
3	A	900	D52	C10-N1	2.80	1.37	1.31
3	A	900	D52	C10-N10	2.70	1.42	1.38
3	A	900	D52	C2A-N3A	2.00	1.35	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	D52	N3A-C2A-N1A	-3.38	123.39	128.68
3	A	900	D52	O4B-C1B-C2B	-2.79	102.85	106.93
3	A	900	D52	C1B-N9A-C4A	-2.54	122.17	126.64
3	A	900	D52	PA-O3P-P	-2.39	124.61	132.83
3	A	900	D52	O4-C4-C4X	-2.26	118.47	121.43
3	A	900	D52	N6A-C6A-N1A	2.01	122.74	118.57
3	A	900	D52	O2A-PA-O1A	2.00	122.15	112.24

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	900	D52	C4X

All (4) torsion outliers are listed below:

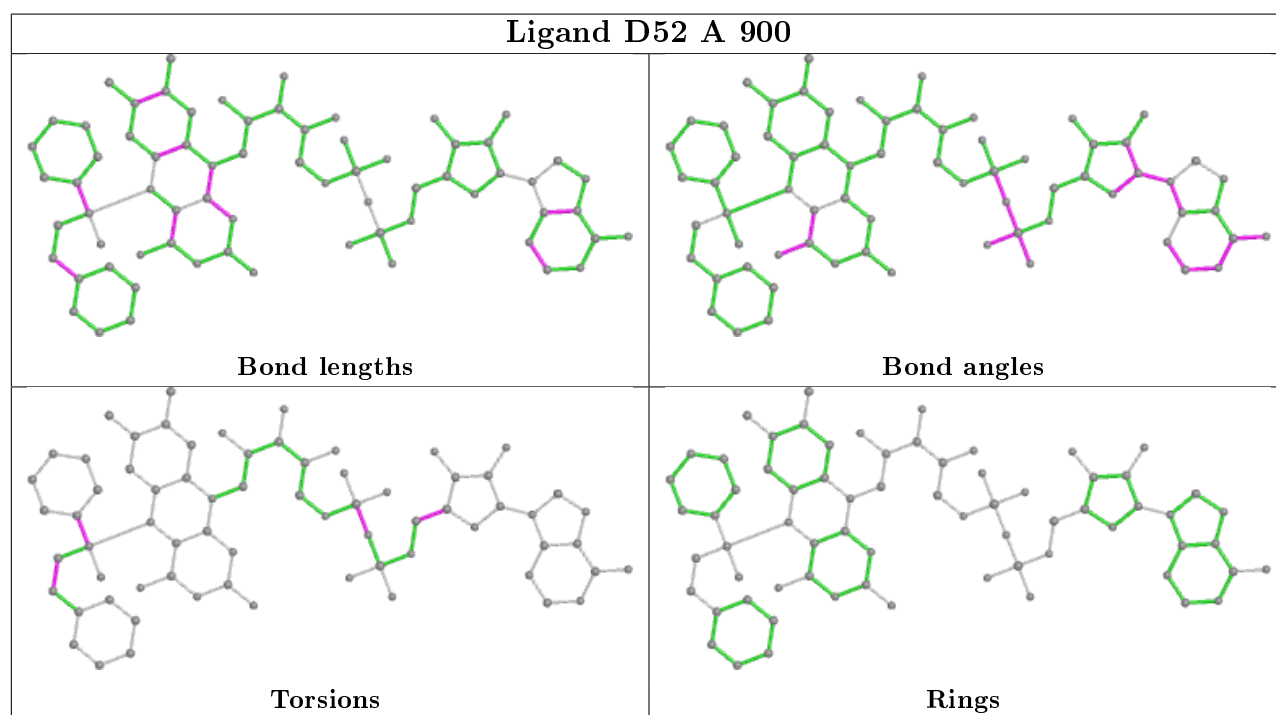
Mol	Chain	Res	Type	Atoms
3	A	900	D52	CAN-CAL-CAM-CAP
3	A	900	D52	CAJ-CAO-CAP-N5
3	A	900	D52	PA-O3P-P-O5'
3	A	900	D52	O4B-C4B-C5B-O5B

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	D52	7	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 [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, 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%)	0.01	5 (0%) 86 72	42, 79, 120, 191	0
2	B	133/482 (27%)	0.22	0 100 100	72, 108, 133, 154	0
All	All	799/1354 (59%)	0.04	5 (0%) 89 78	42, 85, 126, 191	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	835	THR	4.7
1	A	834	TYR	3.0
1	A	504	LEU	2.4
1	A	171	PRO	2.3
1	A	174	VAL	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](#)

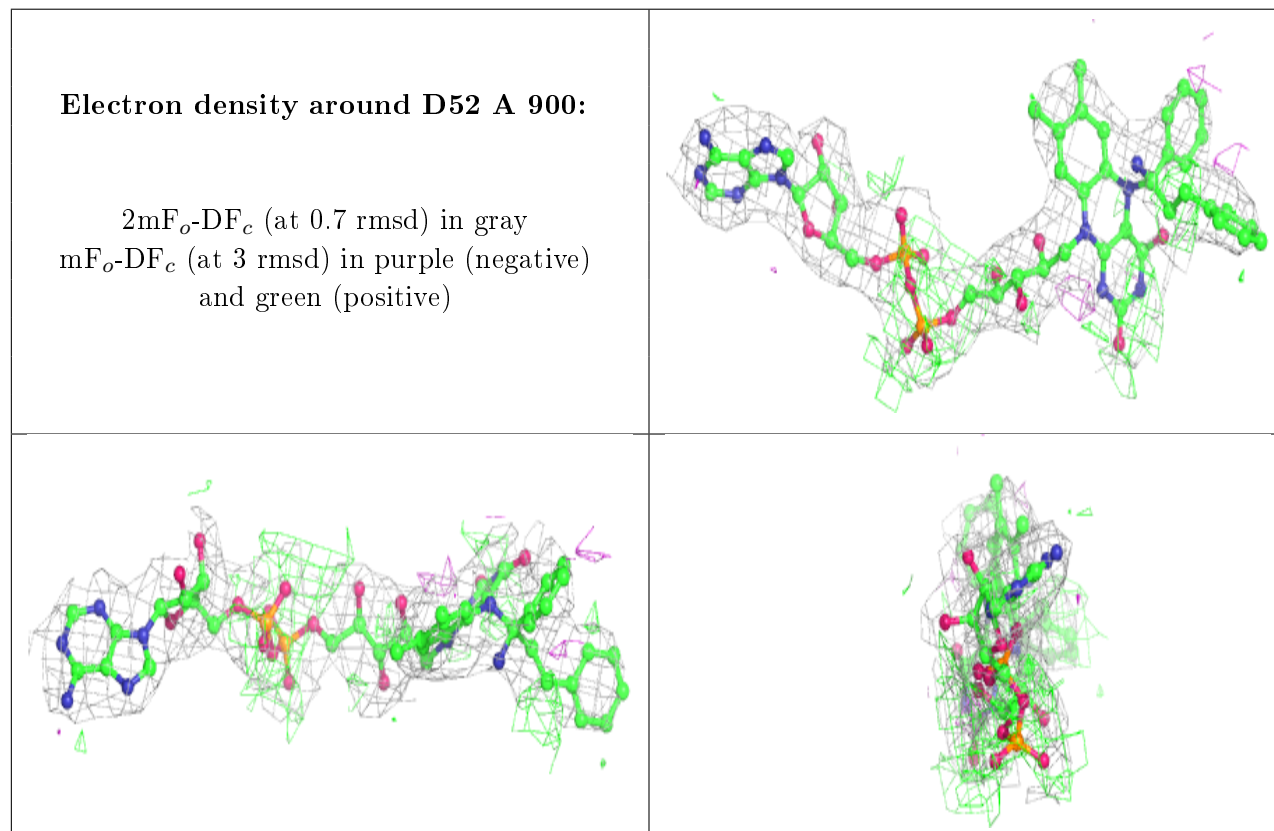
There are no carbohydrates in this entry.

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, 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(\AA^2)	Q<0.9
3	D52	A	900	69/69	0.98	0.24	49,68,111,119	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 ⓘ

There are no such residues in this entry.