



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:46 AM UTC

PDB ID : 4GUU / pdb_00004guu
Title : Crystal structure of LSD2-NPAC with tranylcypromine
Authors : Chen, F.; Dong, Z.; Fang, J.; Yang, Y.; Li, Z.; Xu, Y.; Yang, H.; Wang, P.;
Xu, Y.
Deposited on : 2012-08-29
Resolution : 2.30 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

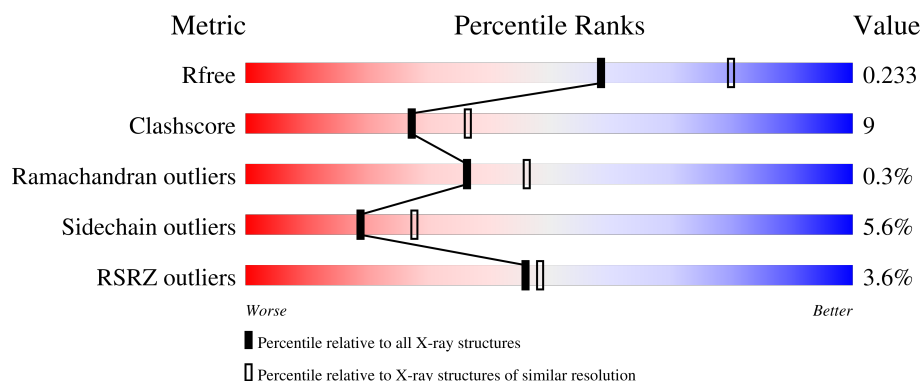
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

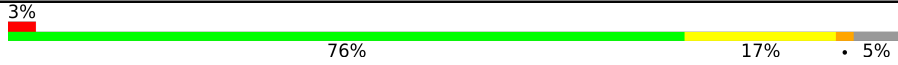
The reported resolution of this entry is 2.30 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	776	
2	B	124	

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	FA9	A	901	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6246 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 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	740	Total	C	N	O	S	0	0	0
			5856	3738	998	1079	41			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	PRO	-	expression tag	UNP Q8NB78
A	48	LEU	-	expression tag	UNP Q8NB78
A	49	GLY	-	expression tag	UNP Q8NB78
A	50	SER	-	expression tag	UNP Q8NB78

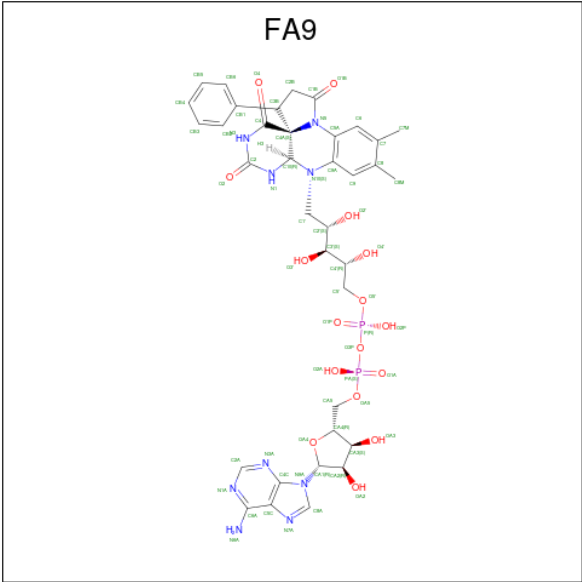
- Molecule 2 is a protein called Putative oxidoreductase GLYR1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	0	0	0
			105	69	19	17			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	145	PRO	-	expression tag	UNP Q49A26
B	146	LEU	-	expression tag	UNP Q49A26
B	147	GLY	-	expression tag	UNP Q49A26
B	148	SER	-	expression tag	UNP Q49A26
B	149	PRO	-	expression tag	UNP Q49A26
B	150	GLU	-	expression tag	UNP Q49A26
B	151	PHE	-	expression tag	UNP Q49A26

- Molecule 3 is [(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methyl (2R,3S,4S)-5-[(3R,3aS,7aR)-10,11-dimethyl-1,4,6-trioxo-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: FA9) (formula: C₃₆H₄₃N₉O₁₆P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			63	36	9	16	2		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Zn	0	0
			3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	216	Total	O	0	0
			216	216		
5	B	3	Total	O	0	0
			3	3		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.82Å 90.16Å 87.82Å 90.00° 104.20° 90.00°	Depositor
Resolution (Å)	36.23 – 2.30 36.23 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.0 (36.23-2.30) 93.4 (36.23-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_353)	Depositor
R, R_{free}	0.199 , 0.231 0.198 , 0.233	Depositor DCC
R_{free} test set	2004 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6246	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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: ZN, FA9

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	0.32	0/6001	0.72	0/8129
2	B	0.36	0/110	1.01	3/149 (2.0%)
All	All	0.33	0/6111	0.73	3/8278 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	216	HIS	N-CA-C	-5.96	105.59	112.92
2	B	214	ASP	CA-C-N	5.25	126.40	119.84
2	B	214	ASP	C-N-CA	5.25	126.40	119.84

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	5856	0	5774	104	0
2	B	105	0	91	4	0
3	A	63	0	40	2	0
4	A	3	0	0	0	0
5	A	216	0	0	4	0
5	B	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6246	0	5905	108	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 9.

All (108) 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:151:ARG:HD2	1:A:169:CYS:SG	2.11	0.90
1:A:454:LEU:HD21	1:A:585:LYS:HG3	1.54	0.88
1:A:267:ARG:CG	1:A:267:ARG:HH11	1.91	0.84
1:A:267:ARG:HH11	1:A:267:ARG:HG3	1.42	0.84
1:A:493:VAL:HG11	1:A:516:ILE:HG21	1.59	0.83
1:A:327:THR:OG1	1:A:330:LYS:HD3	1.90	0.72
1:A:493:VAL:HG13	1:A:516:ILE:HD13	1.70	0.71
1:A:550:ASN:HB3	1:A:553:GLN:HE22	1.55	0.71
1:A:668:TYR:CZ	1:A:747:PRO:HG3	2.25	0.70
1:A:76:ASN:H	1:A:76:ASN:HD22	1.39	0.68
1:A:304:PRO:HB2	1:A:308:LEU:HD22	1.74	0.68
1:A:136:LEU:HD13	1:A:339:GLY:HA3	1.75	0.68
1:A:603:TYR:CZ	1:A:641:PRO:HD2	2.29	0.67
1:A:551:LEU:HA	1:A:554:VAL:HG13	1.84	0.60
1:A:76:ASN:HD22	1:A:76:ASN:N	1.97	0.59
1:A:306:MET:HE3	1:A:345:CYS:HA	1.84	0.58
1:A:204:MET:HA	1:A:204:MET:HE2	1.85	0.58
1:A:76:ASN:H	1:A:76:ASN:ND2	2.01	0.57
1:A:51:ARG:HG2	1:A:51:ARG:HH11	1.70	0.56
1:A:498:ARG:HD2	5:A:1313:HOH:O	2.06	0.56
1:A:149:LYS:HD2	1:A:189:GLU:HB2	1.88	0.56
1:A:722:ARG:HG3	1:A:723:THR:N	2.21	0.56
1:A:495:SER:HA	1:A:498:ARG:HG2	1.88	0.55
1:A:55:LYS:HE3	1:A:204:MET:CE	2.36	0.55
1:A:382:ASN:O	1:A:383:LYS:HB3	2.04	0.55
1:A:131:MET:HE1	1:A:135:GLN:HG3	1.88	0.55
1:A:54:GLU:HG3	1:A:55:LYS:N	2.22	0.55
1:A:296:GLU:HG3	1:A:355:PHE:CE1	2.41	0.54
1:A:603:TYR:CE2	1:A:641:PRO:HD2	2.42	0.54
1:A:120:ASN:HD22	1:A:120:ASN:C	2.16	0.54
1:A:371:ALA:HA	1:A:374:TYR:CZ	2.43	0.54
1:A:279:GLY:HA3	2:B:216:HIS:O	2.08	0.53
1:A:53:CYS:SG	1:A:84:HIS:HB2	2.48	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:TYR:CE2	1:A:747:PRO:HG3	2.43	0.53
1:A:217:ALA:HB3	1:A:218:PRO:HD3	1.90	0.53
1:A:399:ARG:HD3	5:A:1315:HOH:O	2.09	0.53
2:B:219:HIS:CE1	2:B:221:LEU:HB2	2.44	0.52
1:A:92:CYS:SG	1:A:94:GLU:HG2	2.49	0.52
1:A:372:ASP:OD1	1:A:372:ASP:N	2.42	0.52
1:A:727:LYS:O	1:A:731:GLN:HG3	2.09	0.52
1:A:753:PHE:CD1	1:A:753:PHE:C	2.88	0.51
1:A:551:LEU:HA	1:A:554:VAL:CG1	2.41	0.51
1:A:725:ASP:H	1:A:728:GLN:HE21	1.59	0.51
1:A:267:ARG:HD2	5:A:1266:HOH:O	2.10	0.51
1:A:722:ARG:HG3	1:A:723:THR:HG23	1.93	0.51
1:A:131:MET:CE	1:A:135:GLN:HG3	2.41	0.50
1:A:93:ASN:O	1:A:96:PHE:HB3	2.11	0.50
1:A:84:HIS:CD2	1:A:84:HIS:C	2.90	0.50
1:A:377:PRO:HD2	1:A:380:TYR:CE2	2.46	0.50
1:A:52:LYS:HD3	5:A:1182:HOH:O	2.10	0.50
1:A:117:TRP:CD1	1:A:125:PRO:HB3	2.47	0.50
1:A:229:GLY:HA3	1:A:309:ALA:HB2	1.92	0.50
1:A:725:ASP:H	1:A:728:GLN:NE2	2.10	0.49
1:A:267:ARG:HG3	1:A:267:ARG:NH1	2.21	0.49
1:A:719:ALA:O	1:A:722:ARG:HG2	2.13	0.49
1:A:136:LEU:HD13	1:A:339:GLY:CA	2.41	0.49
1:A:55:LYS:HE3	1:A:204:MET:HE1	1.94	0.49
1:A:86:SER:HB3	1:A:205:LEU:HD23	1.95	0.49
1:A:493:VAL:CG1	1:A:516:ILE:HD13	2.39	0.48
1:A:802:PRO:O	1:A:803:GLN:HB2	2.12	0.48
1:A:165:LYS:HB2	1:A:165:LYS:HE3	1.55	0.47
1:A:297:PHE:HB3	1:A:300:TYR:HD2	1.78	0.47
1:A:506:ASP:OD2	1:A:557:ARG:HG3	2.14	0.47
1:A:376:LEU:HB3	1:A:380:TYR:CD2	2.50	0.47
1:A:102:SER:HA	1:A:107:TYR:CD1	2.49	0.47
1:A:267:ARG:CG	1:A:267:ARG:NH1	2.60	0.47
1:A:72:ARG:O	1:A:94:GLU:HG3	2.15	0.46
1:A:725:ASP:CG	1:A:728:GLN:HE21	2.23	0.46
1:A:550:ASN:HD22	1:A:716:GLU:HG3	1.79	0.46
1:A:102:SER:HA	1:A:107:TYR:CG	2.50	0.46
1:A:116:ILE:C	1:A:118:THR:N	2.74	0.45
2:B:214:ASP:C	2:B:216:HIS:H	2.24	0.45
1:A:490:LEU:HD13	1:A:513:ILE:HG23	1.99	0.45
3:A:901:FA9:CB6	3:A:901:FA9:H3	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:TRP:CH2	1:A:507:VAL:HG22	2.53	0.44
1:A:493:VAL:CG1	1:A:516:ILE:HG21	2.41	0.44
1:A:693:LEU:HD22	1:A:694:PHE:CD1	2.52	0.44
1:A:277:GLU:O	2:B:217:PHE:HE1	2.00	0.44
1:A:565:PHE:CD1	1:A:800:HIS:CE1	3.06	0.44
1:A:640:ASN:HA	1:A:641:PRO:C	2.42	0.44
1:A:470:GLU:HA	1:A:471:GLY:HA2	1.56	0.44
1:A:383:LYS:HA	1:A:621:GLN:OE1	2.19	0.43
1:A:693:LEU:HD22	1:A:694:PHE:CE1	2.54	0.43
1:A:85:LEU:HD12	1:A:85:LEU:HA	1.84	0.42
1:A:50:SER:N	1:A:79:THR:O	2.44	0.42
1:A:163:ILE:O	1:A:167:TYR:HB2	2.18	0.42
1:A:375:LEU:HD12	1:A:403:ASN:HB3	2.01	0.42
1:A:525:GLY:O	1:A:526:ILE:C	2.62	0.42
1:A:53:CYS:SG	1:A:55:LYS:HB3	2.59	0.42
1:A:99:TYR:CE2	1:A:131:MET:HE1	2.54	0.42
1:A:144:LYS:HE2	1:A:146:GLU:CG	2.50	0.42
1:A:304:PRO:HB2	1:A:308:LEU:CD2	2.46	0.42
1:A:48:LEU:HD23	1:A:48:LEU:HA	1.74	0.42
1:A:205:LEU:CD1	1:A:207:LEU:O	2.67	0.42
1:A:359:LYS:HB2	1:A:361:LEU:HD23	2.01	0.41
1:A:410:VAL:HG22	1:A:592:ILE:HG23	2.02	0.41
1:A:51:ARG:HH11	1:A:51:ARG:CG	2.33	0.41
1:A:187:LEU:HA	1:A:188:PRO:HD3	1.96	0.41
1:A:222:ALA:HB1	1:A:275:PRO:HG2	2.03	0.41
1:A:85:LEU:O	1:A:205:LEU:HD22	2.20	0.41
1:A:483:MET:HE2	1:A:532:GLU:O	2.21	0.41
1:A:528:PHE:HA	1:A:532:GLU:OE2	2.20	0.41
3:A:901:FA9:H2	3:A:901:FA9:H22	1.85	0.41
1:A:486:HIS:O	1:A:489:ALA:HB3	2.20	0.41
1:A:115:LYS:O	1:A:119:SER:N	2.54	0.41
1:A:693:LEU:HD23	1:A:693:LEU:HA	1.94	0.40
1:A:737:LEU:HD23	1:A:737:LEU:HA	1.91	0.40
1:A:307:TYR:CD2	1:A:307:TYR:C	2.99	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	734/776 (95%)	700 (95%)	33 (4%)	1 (0%)	48	60
2	B	10/124 (8%)	8 (80%)	1 (10%)	1 (10%)	0	0
All	All	744/900 (83%)	708 (95%)	34 (5%)	2 (0%)	36	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	523	GLU
2	B	215	PRO

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	635/662 (96%)	599 (94%)	36 (6%)	18	27
2	B	12/106 (11%)	12 (100%)	0	100	100
All	All	647/768 (84%)	611 (94%)	36 (6%)	19	28

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ARG
1	A	76	ASN
1	A	80	SER
1	A	85	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	94	GLU
1	A	101	ARG
1	A	111	THR
1	A	115	LYS
1	A	116	ILE
1	A	118	THR
1	A	120	ASN
1	A	122	LYS
1	A	146	GLU
1	A	151	ARG
1	A	183	ASP
1	A	267	ARG
1	A	294	LEU
1	A	308	LEU
1	A	344	ARG
1	A	356	MET
1	A	408	VAL
1	A	410	VAL
1	A	430	VAL
1	A	457	SER
1	A	467	LEU
1	A	537	GLN
1	A	554	VAL
1	A	574	LEU
1	A	576	THR
1	A	585	LYS
1	A	680	PHE
1	A	693	LEU
1	A	707	SER
1	A	721	VAL
1	A	730	LEU
1	A	740	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	120	ASN
1	A	141	GLN
1	A	198	ASN
1	A	276	ASN
1	A	440	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	553	GLN
1	A	593	GLN
1	A	609	GLN
1	A	703	GLN
1	A	706	HIS
1	A	728	GLN
1	A	731	GLN
2	B	216	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 [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FA9	A	901	-	64,70,70	2.15	25 (39%)	85,109,109	2.71	26 (30%)

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	FA9	A	901	-	1/1/17/19	4/38/106/106	0/7/8/8

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	FA9	C2B-C3B	-4.99	1.47	1.53
3	A	901	FA9	C5C-N7A	-4.86	1.30	1.39
3	A	901	FA9	C8A-N9A	-4.75	1.29	1.37
3	A	901	FA9	C4-N3	-4.27	1.30	1.37
3	A	901	FA9	C9A-C5A	3.54	1.47	1.41
3	A	901	FA9	C2-N3	-3.53	1.31	1.37
3	A	901	FA9	C9-C8	-3.36	1.35	1.39
3	A	901	FA9	P-O2P	-3.30	1.40	1.55
3	A	901	FA9	P-O1P	-3.28	1.39	1.50
3	A	901	FA9	C4C-N9A	-3.19	1.31	1.37
3	A	901	FA9	CB1-C3B	-3.15	1.47	1.51
3	A	901	FA9	PA-O1A	-2.91	1.40	1.50
3	A	901	FA9	O2-C2	-2.88	1.17	1.23
3	A	901	FA9	C2-N1	-2.81	1.28	1.34
3	A	901	FA9	PA-O2A	-2.73	1.42	1.55
3	A	901	FA9	O4-C4	-2.64	1.18	1.22
3	A	901	FA9	CB6-CB1	-2.44	1.35	1.39
3	A	901	FA9	P-O3P	-2.34	1.57	1.59
3	A	901	FA9	C5C-C4C	2.17	1.43	1.39
3	A	901	FA9	OA4-CA4	-2.16	1.40	1.45
3	A	901	FA9	C5C-C6A	2.15	1.47	1.41
3	A	901	FA9	C5A-N5	-2.14	1.39	1.42
3	A	901	FA9	C1B-N5	-2.08	1.35	1.37
3	A	901	FA9	C8-C7	2.08	1.45	1.40
3	A	901	FA9	C6A-N1A	-2.00	1.30	1.35

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	FA9	C3B-C2B-C1B	-14.94	87.66	104.29
3	A	901	FA9	O1B-C1B-N5	6.48	131.03	125.22
3	A	901	FA9	O1B-C1B-C2B	-6.43	117.86	127.28
3	A	901	FA9	C5C-C4C-N3A	-5.96	118.50	126.72
3	A	901	FA9	N3A-C4C-N9A	5.44	136.42	127.17
3	A	901	FA9	CB2-CB1-C3B	-4.15	112.79	121.07
3	A	901	FA9	C4C-C5C-N7A	-4.02	105.98	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	FA9	C4-N3-C2	-3.94	120.15	126.04
3	A	901	FA9	C4C-N9A-C8A	3.80	109.73	105.74
3	A	901	FA9	C5C-N7A-C8A	3.67	109.22	103.45
3	A	901	FA9	C1'-N10-C9A	-3.39	113.06	120.15
3	A	901	FA9	CB6-CB1-C3B	3.26	127.57	121.07
3	A	901	FA9	C2A-N3A-C4C	3.22	119.69	111.83
3	A	901	FA9	O5'-C5'-C4'	3.09	117.60	109.36
3	A	901	FA9	C9-C9A-N10	-3.04	114.49	120.74
3	A	901	FA9	C6-C5A-C9A	-2.85	115.69	120.06
3	A	901	FA9	N9A-C8A-N7A	-2.80	109.97	113.94
3	A	901	FA9	C2B-C3B-CB1	2.43	122.29	116.84
3	A	901	FA9	O3P-P-O1P	2.36	117.80	110.70
3	A	901	FA9	OA3-CA3-CA4	-2.32	104.43	111.08
3	A	901	FA9	CB4-CB3-CB2	-2.28	117.42	120.24
3	A	901	FA9	O2A-PA-O3P	2.24	113.32	107.27
3	A	901	FA9	O5'-P-O1P	-2.16	100.36	108.94
3	A	901	FA9	C6A-C5C-N7A	2.10	136.15	132.09
3	A	901	FA9	C7M-C7-C8	-2.03	116.61	120.76
3	A	901	FA9	N1A-C2A-N3A	-2.01	125.54	128.58

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	901	FA9	C3B

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	FA9	PA-O3P-P-O5'
3	A	901	FA9	C2B-C3B-CB1-CB2
3	A	901	FA9	C4A-C3B-CB1-CB6
3	A	901	FA9	C4A-C3B-CB1-CB2

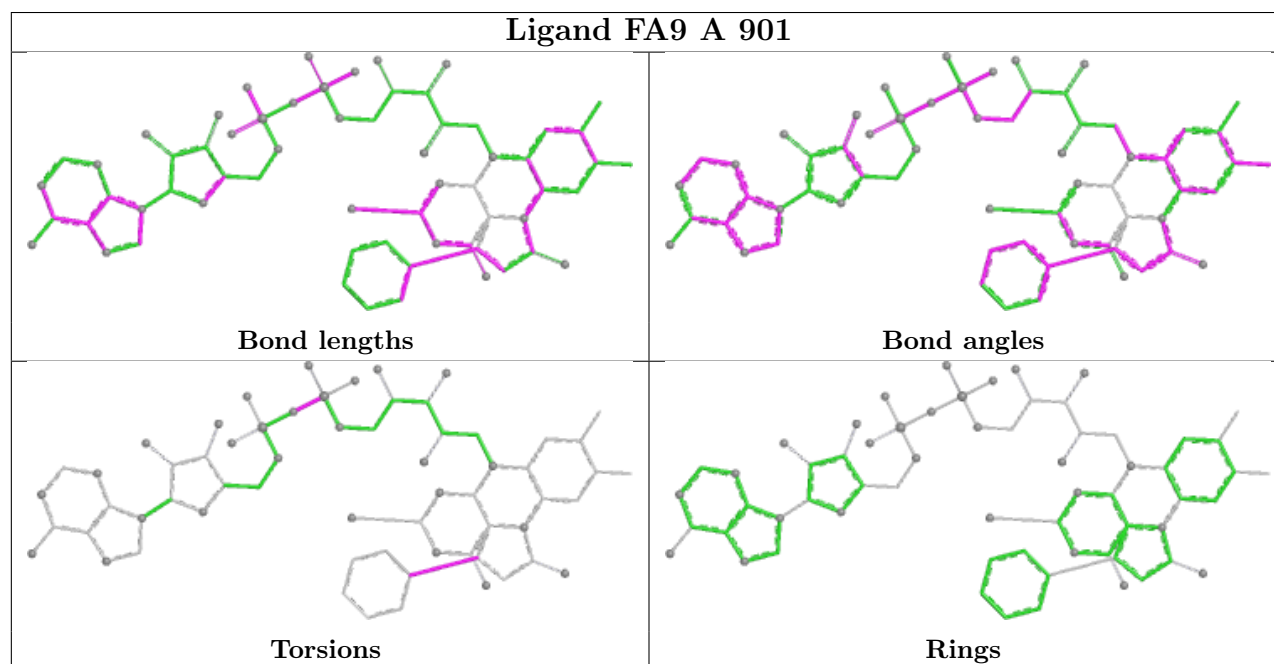
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	FA9	2	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	740/776 (95%)	0.15	22 (2%) 52 54	19, 35, 65, 89	0
2	B	12/124 (9%)	1.42	5 (41%) 0 0	33, 47, 77, 80	0
All	All	752/900 (83%)	0.17	27 (3%) 46 48	19, 36, 65, 89	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	LEU	4.2
1	A	173	PRO	4.2
1	A	47	PRO	4.1
1	A	199	HIS	4.0
2	B	215	PRO	3.6
1	A	200	TRP	3.6
1	A	380	TYR	3.1
2	B	225	THR	3.0
1	A	183	ASP	2.9
1	A	116	ILE	2.7
2	B	216	HIS	2.7
1	A	120	ASN	2.7
1	A	96	PHE	2.6
1	A	121	GLY	2.6
1	A	526	ILE	2.5
1	A	174	ASN	2.5
2	B	217	PHE	2.4
1	A	381	HIS	2.4
1	A	264	GLY	2.3
1	A	60	ALA	2.3
1	A	111	THR	2.3
1	A	82	TRP	2.2
1	A	382	ASN	2.2
1	A	182	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	370	GLY	2.1
1	A	486	HIS	2.1
2	B	218	HIS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

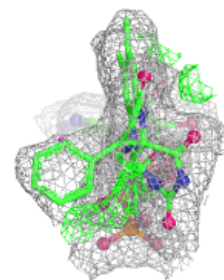
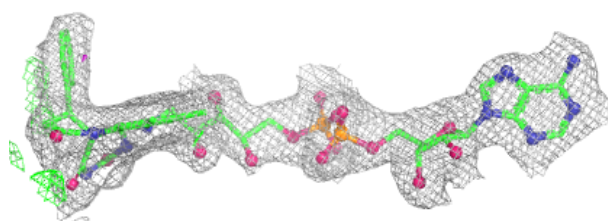
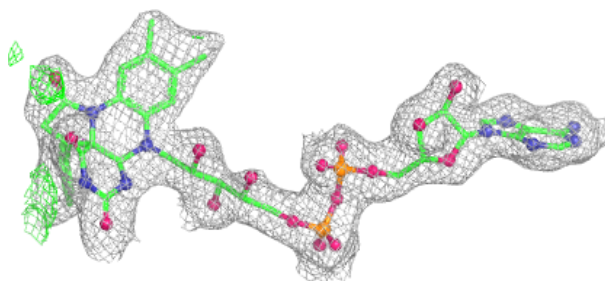
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FA9	A	901	63/63	0.96	0.06	16,25,38,41	0
4	ZN	A	904	1/1	0.98	0.07	40,40,40,40	0
4	ZN	A	903	1/1	0.99	0.03	38,38,38,38	0
4	ZN	A	902	1/1	0.99	0.02	41,41,41,41	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.

Electron density around FA9 A 901:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.