



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:39 am BST

PDB ID : 3ZNN  
Title : IN VITRO AND IN VIVO INHIBITION OF HUMAN D-AMINO ACID OXIDASE: REGULATION OF D-SERINE CONCENTRATION IN THE BRAIN  
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Deposited on : 2013-02-15  
Resolution : 1.90 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

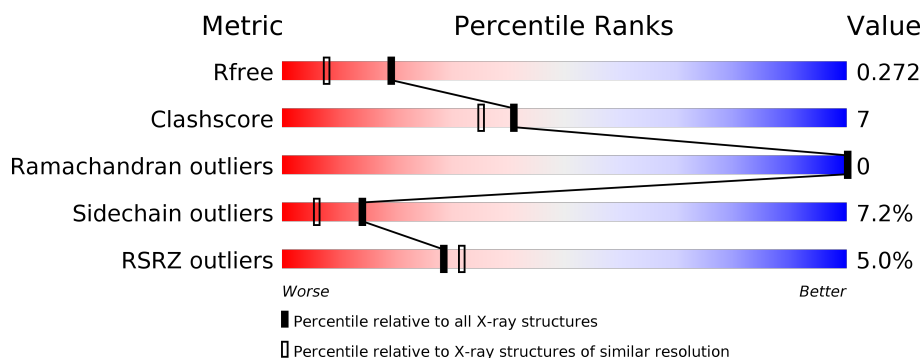
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	347	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>..</div> </div> </div>
1	B	347	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>..</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
4	GOL	A	1341	-	X	-	-
4	GOL	A	1344	-	X	-	-
4	GOL	B	1344	-	-	-	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 6216 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 D-AMINO-ACID OXIDASE.

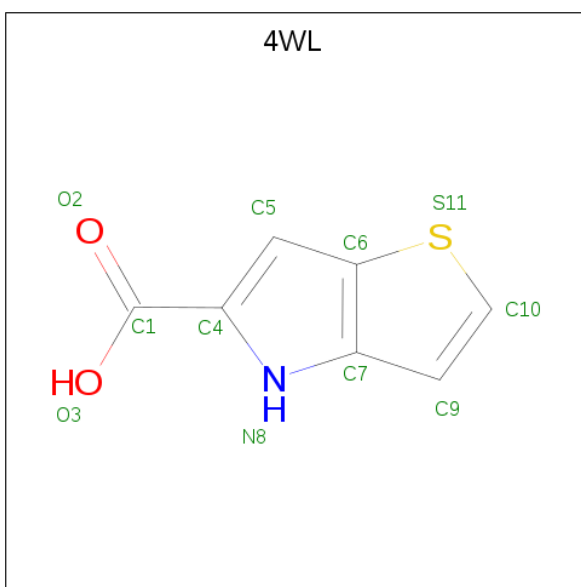
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	10	0
			2789	1790	488	501	10			
1	B	340	Total	C	N	O	S	0	10	0
			2798	1797	492	499	10			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 4H-THIENO[3,2-B]PYROLE-5-CARBOXYLIC ACID (three-letter code: 4WL) (formula: C<sub>7</sub>H<sub>5</sub>NO<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			11	7	1	2	1		
3	B	1	Total	C	N	O	S	0	0
			11	7	1	2	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

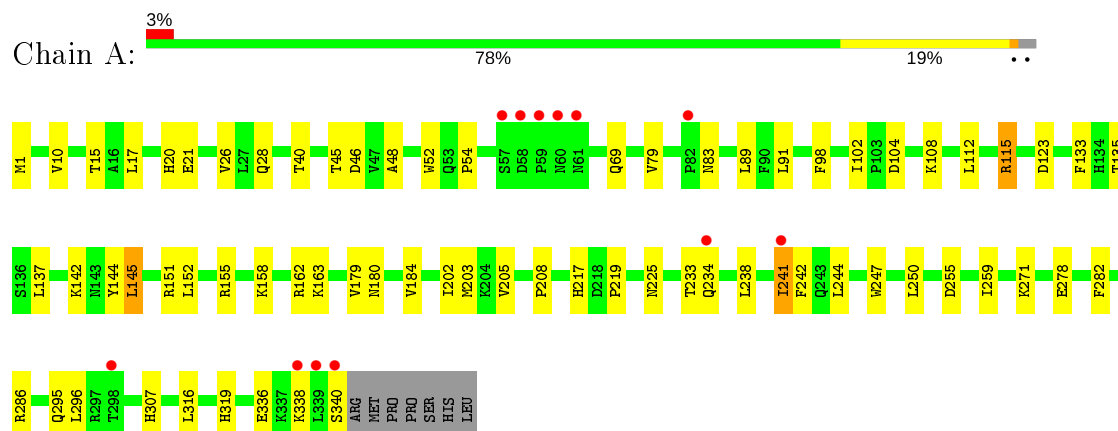
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	219	Total	O	0	25
			244	244		
5	B	168	Total	O	0	23
			191	191		

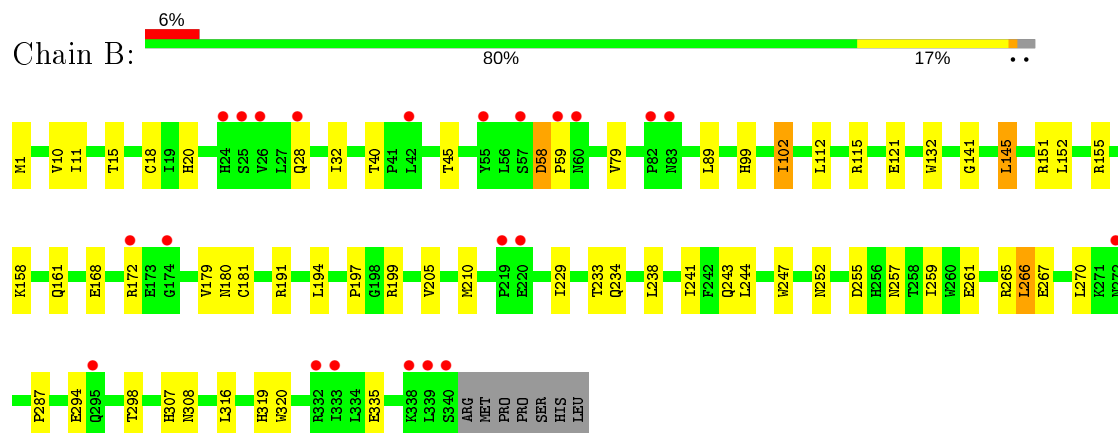
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: D-AMINO-ACID OXIDASE



#### • Molecule 1: D-AMINO-ACID OXIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.83Å 78.68Å 99.96Å 90.00° 92.84° 90.00°	Depositor
Resolution (Å)	15.54 – 1.90 15.45 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.4 (15.54-1.90) 94.4 (15.45-1.90)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 1.90Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, $R_{free}$	0.207 , 0.263 0.213 , 0.272	Depositor DCC
$R_{free}$ test set	2601 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.9	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 59.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6216	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FAD, 4WL

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	0.52	0/2893	0.71	0/3937
1	B	0.49	0/2900	0.69	0/3944
All	All	0.51	0/5793	0.70	0/7881

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	2789	0	2764	41	0
1	B	2798	0	2775	42	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
3	A	11	0	4	0	0
3	B	11	0	4	0	0
4	A	42	0	56	10	0
4	B	24	0	32	9	0
5	A	244	0	0	1	0
5	B	191	0	0	2	0
All	All	6216	0	5697	81	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 7.

All (81) 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:B:99:HIS:HB3	4:B:1343:GOL:H11	1.24	1.15
1:B:180:ASN:HD22	1:B:307:HIS:HD2	1.21	0.89
1:B:241[A]:ILE:HG12	1:B:259[A]:ILE:HD11	1.54	0.87
1:A:241[B]:ILE:HG22	1:A:259:ILE:HD11	1.57	0.86
1:B:287:PRO:HD3	4:B:1341:GOL:H12	1.59	0.85
1:A:180:ASN:HD22	1:A:307:HIS:HD2	1.33	0.77
1:B:191:ARG:HA	4:B:1342:GOL:H11	1.69	0.73
1:B:115:ARG:NH2	1:B:121:GLU:OE1	2.22	0.72
1:A:98:PHE:HB3	4:A:1342:GOL:H11	1.73	0.71
1:A:217:HIS:HE1	4:A:1345:GOL:H11	1.56	0.69
1:B:99:HIS:HA	4:B:1343:GOL:H31	1.73	0.68
1:B:194:LEU:HA	4:B:1341:GOL:H31	1.77	0.67
1:A:217:HIS:CE1	4:A:1345:GOL:H11	2.31	0.66
1:B:316:LEU:O	1:B:319:HIS:HD2	1.78	0.66
1:A:316:LEU:O	1:A:319:HIS:HD2	1.78	0.65
1:B:168:GLU:HG2	1:B:298:THR:HG21	1.82	0.62
1:B:287:PRO:HD3	4:B:1341:GOL:C1	2.30	0.60
1:A:91:LEU:HD23	1:A:137:LEU:HD23	1.86	0.57
1:B:180:ASN:HD22	1:B:307:HIS:CD2	2.12	0.57
1:B:199:ARG:HH11	1:B:243:GLN:HE22	1.51	0.56
1:B:233[A]:THR:HG23	1:B:234:GLN:HG2	1.86	0.56
1:B:191:ARG:HG3	4:B:1342:GOL:H31	1.87	0.55
1:A:104:ASP:HB3	1:A:108:LYS:HD3	1.89	0.55
1:B:191:ARG:HG3	4:B:1342:GOL:H12	1.89	0.54
1:A:17:LEU:O	1:A:21:GLU:HG2	2.07	0.53
1:A:158:LYS:HA	4:A:1341:GOL:H11	1.90	0.53
1:A:79[B]:VAL:HG11	1:A:137:LEU:CD2	2.39	0.53
1:B:210:MET:CE	1:B:267:GLU:HG2	2.39	0.53
1:B:252:ASN:HD22	1:B:255:ASP:H	1.57	0.52
1:A:219:PRO:HD3	4:A:1342:GOL:H2	1.91	0.52
1:A:46:ASP:HB3	1:A:142:LYS:HE2	1.91	0.52
1:B:99:HIS:CB	4:B:1343:GOL:H11	2.16	0.51
1:A:208:PRO:HB2	1:B:233[A]:THR:O	2.10	0.51
1:B:141:GLY:O	1:B:145:LEU:HB2	2.11	0.51
1:A:163:LYS:HD2	4:A:1343:GOL:H11	1.93	0.50
1:B:241[A]:ILE:HG12	1:B:259[A]:ILE:CD1	2.35	0.50
1:A:247:TRP:CE3	4:A:1346:GOL:H31	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASN:HD22	1:A:241[B]:ILE:HA	1.77	0.49
1:B:15:THR:HG21	1:B:179:VAL:HG11	1.94	0.49
1:B:59:PRO:HB3	5:B:2153:HOH:O	2.13	0.48
1:A:225:ASN:HD22	1:A:241[A]:ILE:HA	1.78	0.47
1:A:112:LEU:HB2	1:A:135:THR:HB	1.96	0.47
1:A:162:ARG:O	2:A:350:FAD:H2A	2.15	0.47
1:B:168:GLU:HG2	1:B:298:THR:CG2	2.45	0.47
1:B:40:THR:HB	1:B:145:LEU:HD23	1.97	0.47
1:A:202:ILE:O	1:A:278[A]:GLU:HG3	2.15	0.46
1:B:20:HIS:CE1	1:B:155:ARG:HB3	2.51	0.46
1:A:225:ASN:ND2	1:A:242:PHE:H	2.13	0.46
1:B:11:ILE:HG22	1:B:181:CYS:SG	2.56	0.46
1:A:180:ASN:HD22	1:A:307:HIS:CD2	2.23	0.46
1:A:144:TYR:OH	1:A:319:HIS:HE1	1.99	0.45
1:A:48:ALA:O	4:A:1344:GOL:H32	2.16	0.45
1:A:123:ASP:OD2	5:A:2167:HOH:O	2.21	0.45
1:B:210:MET:HE1	1:B:267:GLU:HG2	1.98	0.45
1:A:98:PHE:CB	4:A:1342:GOL:H11	2.45	0.45
1:B:172[B]:ARG:HA	1:B:172[B]:ARG:HD3	1.81	0.45
1:A:255:ASP:O	1:A:259:ILE:HG12	2.16	0.44
1:B:229:ILE:HD12	1:B:266:LEU:HD13	2.00	0.44
1:A:46:ASP:HA	4:A:1344:GOL:H31	2.00	0.44
1:A:15:THR:HG21	1:A:179:VAL:HG11	2.00	0.44
1:A:10:VAL:HB	1:A:45:THR:HG21	2.00	0.44
1:A:233[A]:THR:HG23	1:A:234:GLN:HG2	2.00	0.43
1:A:184:VAL:HG11	1:A:282:PHE:HB2	2.01	0.43
1:B:197:PRO:HG3	1:B:247:TRP:CE2	2.54	0.43
1:B:199:ARG:HH11	1:B:243:GLN:NE2	2.15	0.42
1:A:203:MET:HG2	1:A:278[B]:GLU:HG2	2.00	0.42
1:B:20:HIS:HD2	1:B:32:ILE:HD12	1.84	0.42
1:B:18[B]:CYS:SG	1:B:320:TRP:CH2	3.11	0.42
1:B:58:ASP:HB2	5:B:2113:HOH:O	2.19	0.42
1:A:91:LEU:HD23	1:A:137:LEU:CD2	2.50	0.42
1:B:102:ILE:HD11	1:B:132:TRP:CZ2	2.54	0.42
1:B:294:GLU:OE1	1:B:307:HIS:HE1	2.03	0.42
1:B:11:ILE:HG21	1:B:308:ASN:O	2.19	0.42
1:A:40:THR:HB	1:A:145:LEU:HD23	2.01	0.41
1:A:208:PRO:HB2	1:B:233[B]:THR:O	2.20	0.41
1:B:199:ARG:NH1	1:B:243:GLN:HE22	2.16	0.41
1:A:336:GLU:C	1:A:338:LYS:H	2.24	0.41
1:A:20:HIS:CE1	1:A:155:ARG:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:TRP:CZ3	1:A:54:PRO:HD3	2.56	0.40
1:B:10:VAL:HB	1:B:45:THR:HG21	2.02	0.40
1:A:115[A]:ARG:NE	1:A:133:PHE:HB3	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	348/347 (100%)	335 (96%)	13 (4%)	0	100	100
1	B	348/347 (100%)	334 (96%)	14 (4%)	0	100	100
All	All	696/694 (100%)	669 (96%)	27 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	302/299 (101%)	278 (92%)	24 (8%)	12	5
1	B	302/299 (101%)	281 (93%)	21 (7%)	15	7
All	All	604/598 (101%)	559 (92%)	45 (8%)	14	5

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	26	VAL
1	A	28[A]	GLN
1	A	28[B]	GLN
1	A	69	GLN
1	A	83	ASN
1	A	89	LEU
1	A	102	ILE
1	A	115[A]	ARG
1	A	115[B]	ARG
1	A	145	LEU
1	A	151	ARG
1	A	152	LEU
1	A	205	VAL
1	A	238	LEU
1	A	241[A]	ILE
1	A	241[B]	ILE
1	A	244	LEU
1	A	250	LEU
1	A	271	LYS
1	A	286	ARG
1	A	295	GLN
1	A	296	LEU
1	A	340	SER
1	B	1	MET
1	B	28	GLN
1	B	58	ASP
1	B	79	VAL
1	B	89	LEU
1	B	102	ILE
1	B	112	LEU
1	B	145	LEU
1	B	151	ARG
1	B	152	LEU
1	B	158	LYS
1	B	161	GLN
1	B	205	VAL
1	B	238	LEU
1	B	244	LEU
1	B	257	ASN
1	B	261	GLU
1	B	265	ARG
1	B	266	LEU

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Mol	Chain	Res	Type
1	B	270	LEU
1	B	335	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	225	ASN
1	A	243	GLN
1	A	307	HIS
1	A	319	HIS
1	B	201	GLN
1	B	225	ASN
1	B	243	GLN
1	B	252	ASN
1	B	307	HIS
1	B	319	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	GOL	A	1346	-	5,5,5	0.70	0	5,5,5	0.29	0
4	GOL	B	1344	-	5,5,5	1.04	0	5,5,5	1.04	0
4	GOL	B	1343	-	5,5,5	0.46	0	5,5,5	1.50	1 (20%)
4	GOL	A	1343	-	5,5,5	0.65	0	5,5,5	1.22	0
4	GOL	A	1347	-	5,5,5	0.98	0	5,5,5	0.83	0
2	FAD	A	350	-	51,58,58	3.66	24 (47%)	60,89,89	3.71	27 (45%)
3	4WL	A	360	-	9,12,12	3.15	2 (22%)	4,17,17	3.71	1 (25%)
4	GOL	B	1342	-	5,5,5	0.83	0	5,5,5	1.50	2 (40%)
4	GOL	A	1344	-	5,5,5	1.57	1 (20%)	5,5,5	2.05	3 (60%)
4	GOL	A	1345	-	5,5,5	1.01	0	5,5,5	1.10	0
4	GOL	B	1341	-	5,5,5	0.65	0	5,5,5	1.10	0
4	GOL	A	1341	-	5,5,5	1.20	1 (20%)	5,5,5	1.58	2 (40%)
3	4WL	B	360	-	9,12,12	2.88	2 (22%)	4,17,17	3.35	1 (25%)
4	GOL	A	1342	-	5,5,5	0.83	0	5,5,5	1.03	0
2	FAD	B	350	-	51,58,58	3.45	20 (39%)	60,89,89	2.91	22 (36%)

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
4	GOL	A	1346	-	-	1/4/4/4	-
4	GOL	B	1344	-	-	0/4/4/4	-
4	GOL	B	1343	-	-	2/4/4/4	-
4	GOL	A	1343	-	-	4/4/4/4	-
4	GOL	A	1347	-	-	4/4/4/4	-
2	FAD	A	350	-	-	2/30/50/50	0/6/6/6
3	4WL	A	360	-	-	0/0/4/4	0/2/2/2
4	GOL	B	1342	-	-	2/4/4/4	-
4	GOL	A	1344	-	-	2/4/4/4	-
4	GOL	A	1345	-	-	3/4/4/4	-
4	GOL	B	1341	-	-	2/4/4/4	-
4	GOL	A	1341	-	-	4/4/4/4	-
3	4WL	B	360	-	-	0/0/4/4	0/2/2/2
4	GOL	A	1342	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	350	-	-	3/30/50/50	0/6/6/6

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	350	FAD	C4X-C10	13.42	1.52	1.38
2	A	350	FAD	C4X-C10	10.46	1.49	1.38
2	A	350	FAD	C5'-C4'	9.73	1.65	1.51
2	A	350	FAD	O4B-C1B	9.05	1.53	1.41
3	A	360	4WL	C6-S11	-8.61	1.67	1.74
3	B	360	4WL	C6-S11	-7.75	1.68	1.74
2	B	350	FAD	O4B-C1B	7.47	1.51	1.41
2	A	350	FAD	C1'-N10	7.47	1.55	1.48
2	B	350	FAD	C5'-C4'	7.18	1.62	1.51
2	A	350	FAD	C2'-C3'	7.06	1.66	1.53
2	B	350	FAD	C4X-N5	6.87	1.43	1.33
2	A	350	FAD	C4X-N5	6.85	1.43	1.33
2	B	350	FAD	C10-N1	6.29	1.41	1.33
2	B	350	FAD	C2A-N3A	6.16	1.42	1.32
2	B	350	FAD	C9A-C5X	5.77	1.54	1.42
2	A	350	FAD	C9A-C5X	4.59	1.51	1.42
2	A	350	FAD	C10-N1	4.57	1.39	1.33
2	B	350	FAD	C2A-N1A	4.53	1.42	1.33
2	A	350	FAD	C2A-N1A	4.32	1.41	1.33
2	A	350	FAD	C2A-N3A	4.22	1.38	1.32
2	A	350	FAD	C6-C5X	-4.02	1.35	1.41
2	B	350	FAD	O3'-C3'	4.00	1.52	1.43
2	A	350	FAD	O3'-C3'	3.99	1.52	1.43
2	B	350	FAD	C1'-N10	3.90	1.52	1.48
2	A	350	FAD	C4-N3	3.81	1.39	1.33
2	A	350	FAD	O3B-C3B	3.81	1.51	1.43
2	B	350	FAD	C2'-C3'	3.65	1.60	1.53
2	A	350	FAD	O2'-C2'	3.65	1.51	1.43
2	A	350	FAD	C9-C8	3.48	1.46	1.37
2	B	350	FAD	C4-N3	3.45	1.39	1.33
2	A	350	FAD	C9A-N10	-3.45	1.33	1.38
2	B	350	FAD	O3B-C3B	3.37	1.50	1.43
3	A	360	4WL	C7-C6	-3.01	1.32	1.42
2	B	350	FAD	C6-C5X	-3.00	1.37	1.41
2	A	350	FAD	P-O2P	-2.84	1.42	1.55
3	B	360	4WL	C7-C6	-2.75	1.33	1.42
2	B	350	FAD	O4B-C4B	2.63	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	350	FAD	PA-O5B	2.52	1.69	1.59
2	B	350	FAD	C2B-C1B	-2.45	1.50	1.53
2	B	350	FAD	C8-C7	2.40	1.46	1.40
4	A	1341	GOL	O3-C3	2.31	1.52	1.42
2	A	350	FAD	C6-C7	2.25	1.43	1.37
2	B	350	FAD	C6-C7	2.18	1.43	1.37
4	A	1344	GOL	C1-C2	2.17	1.60	1.51
2	B	350	FAD	PA-O1A	-2.15	1.43	1.50
2	A	350	FAD	C2-N3	2.14	1.42	1.38
2	A	350	FAD	O4-C4	2.12	1.29	1.24
2	A	350	FAD	C5A-C4A	2.03	1.46	1.40
2	A	350	FAD	O4'-C4'	-2.01	1.39	1.43
2	B	350	FAD	P-O5'	2.01	1.67	1.59

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	350	FAD	C1'-N10-C9A	14.07	129.37	118.29
2	A	350	FAD	C1'-N10-C10	-9.66	109.76	118.41
2	B	350	FAD	C1'-N10-C9A	8.89	125.29	118.29
2	A	350	FAD	N3A-C2A-N1A	-7.75	116.57	128.68
3	A	360	4WL	C5-C6-C7	7.25	112.55	106.24
2	A	350	FAD	C4-C4X-N5	7.02	126.62	118.60
2	A	350	FAD	C4X-N5-C5X	6.95	123.72	116.77
2	B	350	FAD	N3A-C2A-N1A	-6.94	117.83	128.68
2	B	350	FAD	C4-C4X-C10	-6.91	115.38	119.95
3	B	360	4WL	C5-C6-C7	6.67	112.04	106.24
2	A	350	FAD	C4-C4X-C10	-6.21	115.84	119.95
2	B	350	FAD	C5X-C9A-N10	5.90	121.99	117.72
2	B	350	FAD	C4-N3-C2	5.89	120.12	115.14
2	A	350	FAD	O5B-C5B-C4B	-5.49	90.09	108.99
2	A	350	FAD	C10-C4X-N5	-5.40	117.52	121.26
2	A	350	FAD	O4'-C4'-C3'	-4.86	97.28	109.10
2	A	350	FAD	C5X-C9A-N10	4.82	121.21	117.72
2	B	350	FAD	O5B-C5B-C4B	-4.76	92.60	108.99
2	B	350	FAD	C4-C4X-N5	4.62	123.88	118.60
2	A	350	FAD	C2A-N1A-C6A	4.59	126.61	118.75
2	A	350	FAD	C3B-C2B-C1B	-4.59	94.07	100.98
2	B	350	FAD	C5'-C4'-C3'	-4.55	103.42	112.20
2	B	350	FAD	C4X-N5-C5X	4.46	121.22	116.77
2	B	350	FAD	C4A-C5A-N7A	-4.45	104.76	109.40
2	B	350	FAD	C1'-N10-C10	-4.30	114.56	118.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	350	FAD	C5'-C4'-C3'	-4.21	104.06	112.20
2	A	350	FAD	O5'-C5'-C4'	-4.18	98.20	109.36
2	B	350	FAD	O5'-C5'-C4'	-4.01	98.66	109.36
2	A	350	FAD	C4-N3-C2	3.85	118.39	115.14
2	A	350	FAD	C4A-C5A-N7A	-3.80	105.44	109.40
2	A	350	FAD	O3'-C3'-C4'	-3.51	100.34	108.81
2	A	350	FAD	O5B-PA-O1A	-3.39	95.83	109.07
2	A	350	FAD	C4'-C3'-C2'	-3.35	106.39	113.36
2	B	350	FAD	C3B-C2B-C1B	-3.30	96.01	100.98
2	B	350	FAD	C4X-C10-N10	-3.23	116.98	120.30
2	B	350	FAD	O4B-C4B-C5B	-3.20	98.86	109.37
2	B	350	FAD	C2A-N1A-C6A	3.10	124.06	118.75
2	A	350	FAD	C6-C5X-C9A	2.95	122.92	119.05
2	A	350	FAD	O2'-C2'-C3'	-2.82	102.23	109.10
2	B	350	FAD	O4'-C4'-C5'	-2.77	103.68	109.92
4	A	1344	GOL	O1-C1-C2	2.67	123.02	110.20
2	A	350	FAD	C9A-C5X-N5	-2.61	118.28	122.36
4	A	1344	GOL	C3-C2-C1	2.58	121.73	111.70
2	A	350	FAD	C1'-C2'-C3'	-2.48	102.85	109.79
2	A	350	FAD	O3'-C3'-C2'	2.31	114.40	108.81
2	B	350	FAD	C9A-C5X-N5	-2.29	118.77	122.36
2	B	350	FAD	C4'-C3'-C2'	-2.26	108.67	113.36
2	B	350	FAD	C2B-C3B-C4B	2.25	107.02	102.64
4	A	1344	GOL	O2-C2-C3	-2.24	99.25	109.12
4	B	1343	GOL	O1-C1-C2	2.20	120.76	110.20
2	B	350	FAD	C8M-C8-C7	2.19	125.22	120.74
2	A	350	FAD	P-O3P-PA	-2.16	125.40	132.83
2	A	350	FAD	C9-C9A-C5X	-2.13	116.25	119.88
2	B	350	FAD	C1'-C2'-C3'	-2.12	103.87	109.79
4	B	1342	GOL	C3-C2-C1	-2.07	103.66	111.70
2	A	350	FAD	C8M-C8-C7	2.03	124.89	120.74
4	A	1341	GOL	O2-C2-C3	2.02	118.03	109.12
4	B	1342	GOL	O1-C1-C2	2.02	119.89	110.20
4	A	1341	GOL	C3-C2-C1	2.02	119.54	111.70

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1343	GOL	C1-C2-C3-O3
4	A	1347	GOL	O1-C1-C2-C3
4	A	1347	GOL	C1-C2-C3-O3

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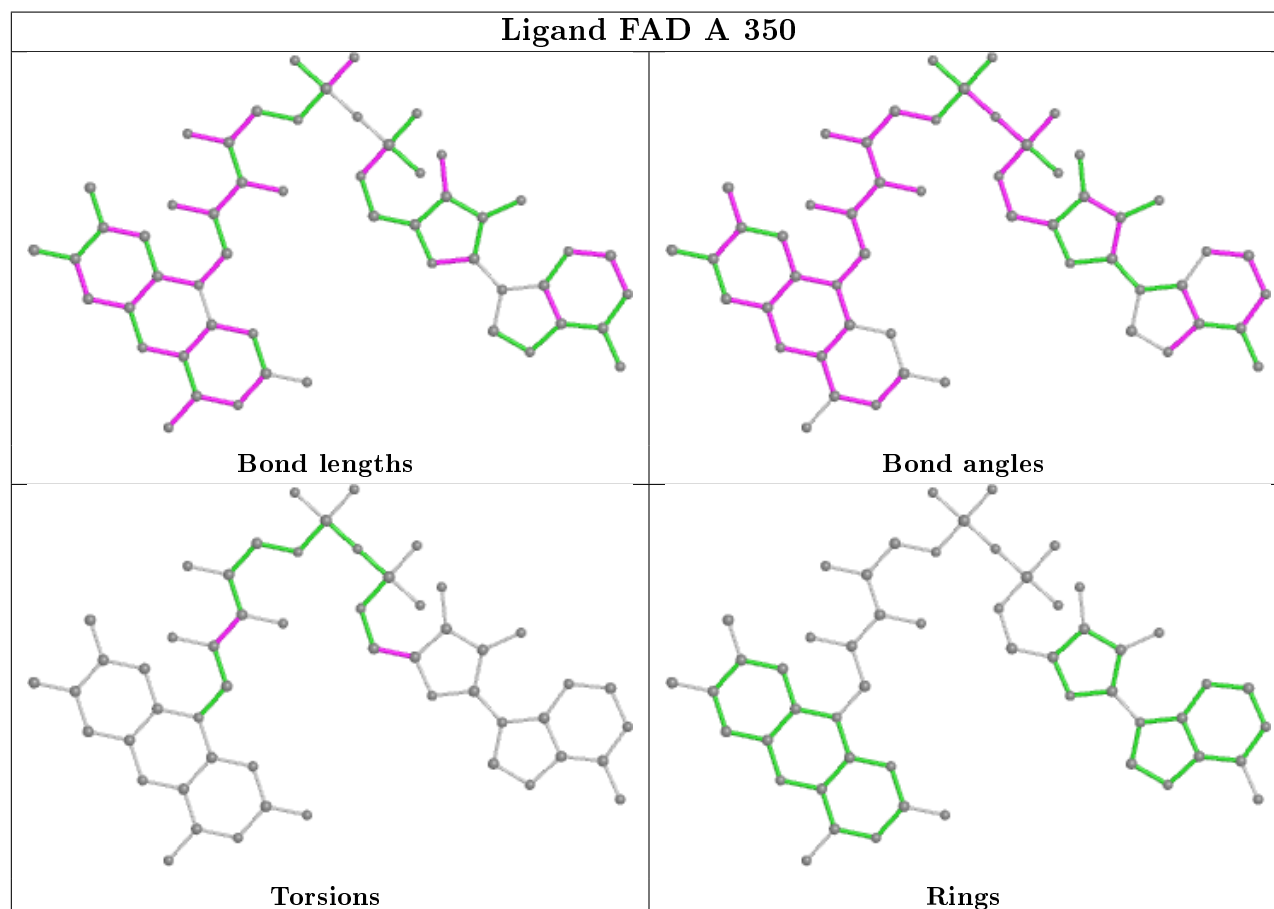
Mol	Chain	Res	Type	Atoms
4	B	1342	GOL	O1-C1-C2-C3
4	A	1345	GOL	O1-C1-C2-C3
4	B	1341	GOL	C1-C2-C3-O3
4	A	1341	GOL	O1-C1-C2-C3
4	A	1341	GOL	O2-C2-C3-O3
2	A	350	FAD	O2'-C2'-C3'-C4'
4	A	1347	GOL	O1-C1-C2-O2
4	B	1343	GOL	O1-C1-C2-C3
4	A	1343	GOL	O1-C1-C2-C3
4	A	1344	GOL	C1-C2-C3-O3
4	A	1345	GOL	C1-C2-C3-O3
4	A	1341	GOL	C1-C2-C3-O3
4	B	1343	GOL	O1-C1-C2-O2
4	A	1347	GOL	O2-C2-C3-O3
4	B	1342	GOL	O1-C1-C2-O2
2	B	350	FAD	O2'-C2'-C3'-C4'
4	A	1341	GOL	O1-C1-C2-O2
4	A	1344	GOL	O2-C2-C3-O3
4	B	1341	GOL	O2-C2-C3-O3
4	A	1343	GOL	O1-C1-C2-O2
4	A	1343	GOL	O2-C2-C3-O3
4	A	1345	GOL	O2-C2-C3-O3
4	A	1346	GOL	C1-C2-C3-O3
4	A	1342	GOL	O1-C1-C2-C3
2	A	350	FAD	O4B-C4B-C5B-O5B
2	B	350	FAD	O4B-C4B-C5B-O5B
2	B	350	FAD	C3B-C4B-C5B-O5B

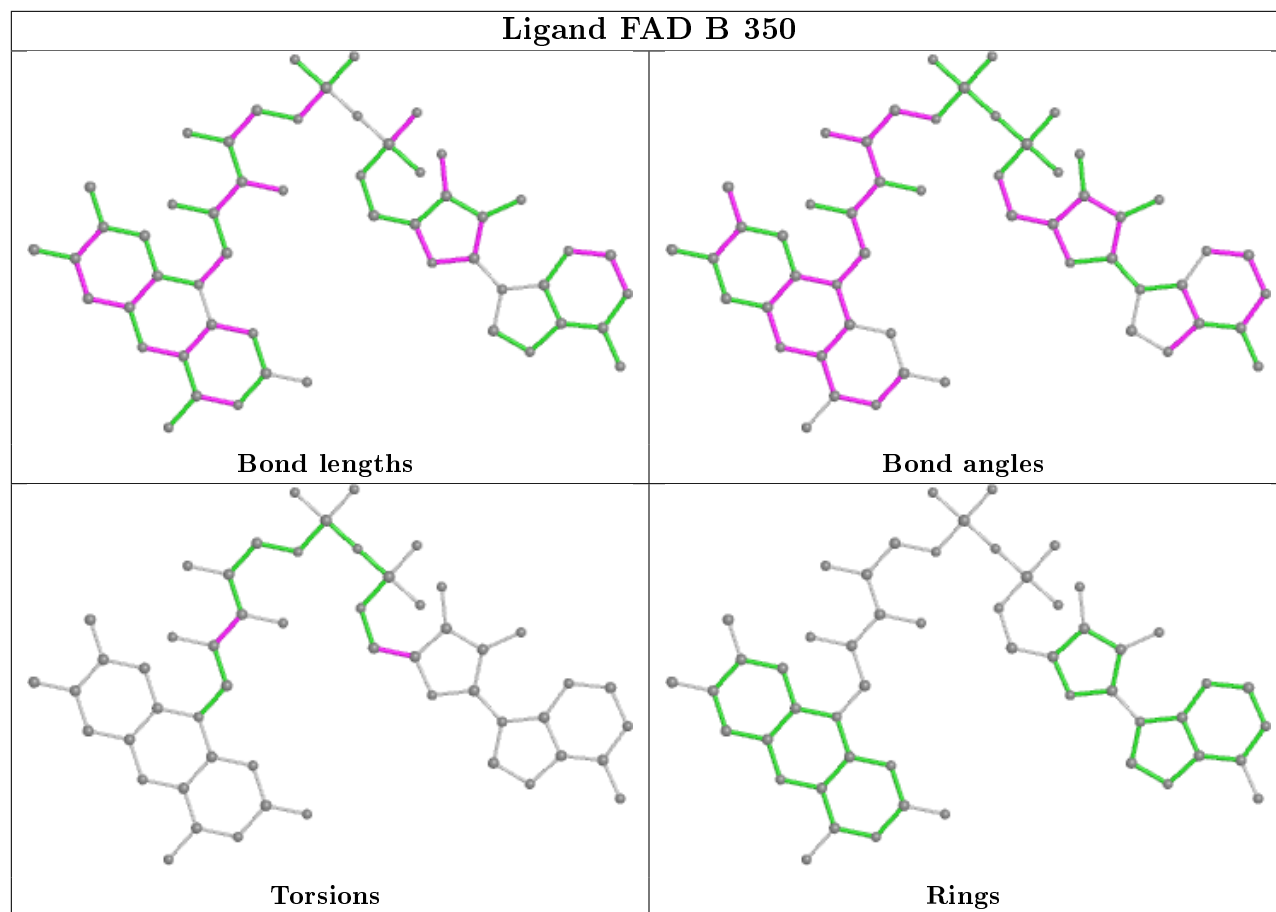
There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1346	GOL	1	0
4	B	1343	GOL	3	0
4	A	1343	GOL	1	0
2	A	350	FAD	1	0
4	B	1342	GOL	3	0
4	A	1344	GOL	2	0
4	A	1345	GOL	2	0
4	B	1341	GOL	3	0
4	A	1341	GOL	1	0
4	A	1342	GOL	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	340/347 (97%)	0.15	12 (3%) 44 47	23, 34, 60, 94	0
1	B	340/347 (97%)	0.43	22 (6%) 18 21	26, 40, 67, 122	0
All	All	680/694 (97%)	0.29	34 (5%) 28 32	23, 37, 66, 122	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	339	LEU	13.5
1	B	339	LEU	11.8
1	B	340	SER	10.7
1	A	60	ASN	9.4
1	B	26	VAL	8.8
1	B	60	ASN	5.9
1	A	59	PRO	5.3
1	A	58	ASP	5.0
1	B	338	LYS	4.7
1	A	338	LYS	4.4
1	A	340	SER	4.4
1	B	82	PRO	4.2
1	B	59	PRO	3.6
1	B	220	GLU	3.5
1	B	42	LEU	3.5
1	A	57	SER	3.1
1	B	28	GLN	3.1
1	B	172[A]	ARG	2.8
1	B	55	TYR	2.8
1	B	25	SER	2.4
1	B	83	ASN	2.3
1	B	333	ILE	2.3
1	B	57	SER	2.2
1	A	234	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	82	PRO	2.2
1	B	332	ARG	2.2
1	B	174	GLY	2.1
1	B	295	GLN	2.1
1	A	61	ASN	2.1
1	A	241[A]	ILE	2.1
1	B	272	ASN	2.0
1	B	24	HIS	2.0
1	B	219	PRO	2.0
1	A	298	THR	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.

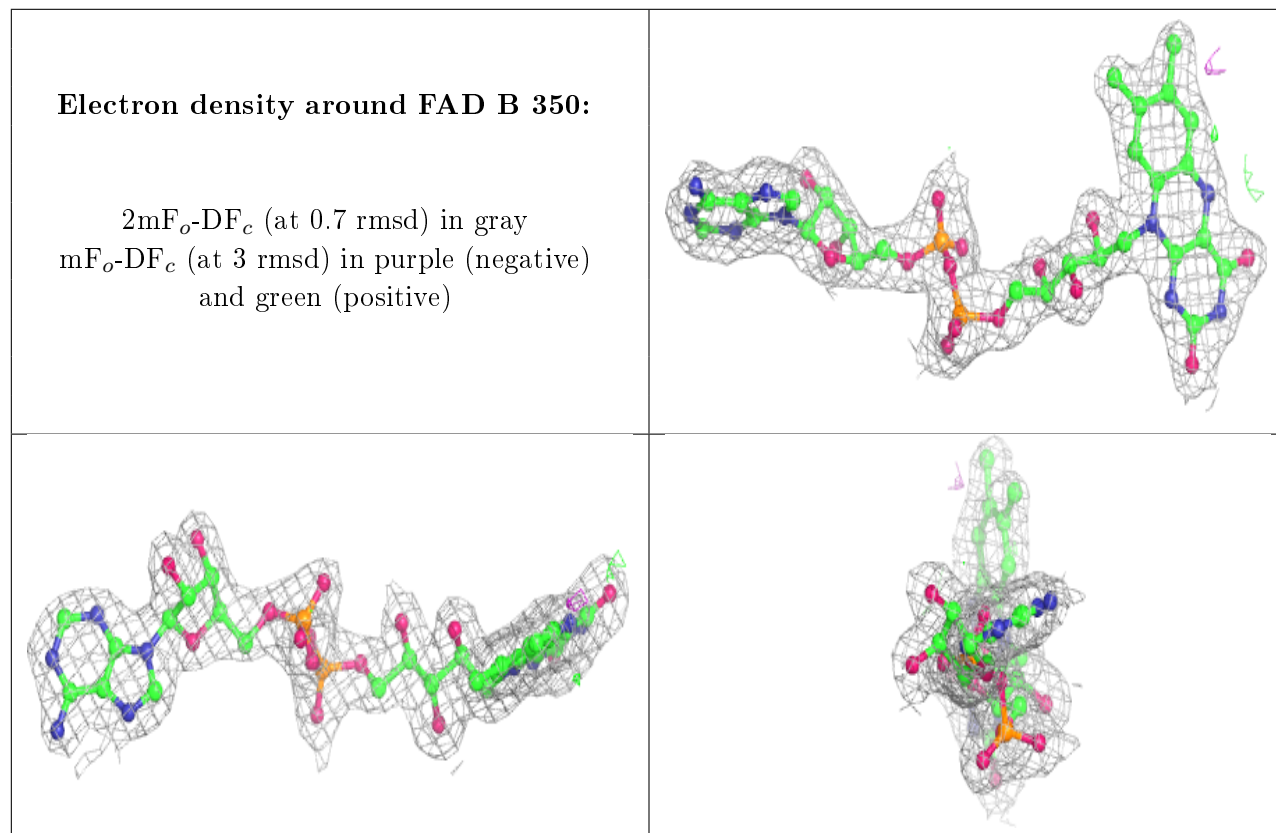
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	A	1347	6/6	0.52	0.38	49,56,57,58	0
4	GOL	B	1344	6/6	0.56	0.45	54,56,57,57	0
4	GOL	B	1341	6/6	0.59	0.37	58,59,60,61	0
4	GOL	A	1346	6/6	0.76	0.25	57,60,61,61	0
4	GOL	A	1341	6/6	0.77	0.25	47,50,51,52	0
4	GOL	A	1345	6/6	0.81	0.20	54,56,56,56	0
4	GOL	A	1342	6/6	0.81	0.24	53,56,56,57	0
4	GOL	A	1344	6/6	0.83	0.19	42,45,47,47	0
4	GOL	B	1342	6/6	0.86	0.29	41,44,45,47	0
4	GOL	A	1343	6/6	0.88	0.28	70,71,71,71	0
4	GOL	B	1343	6/6	0.89	0.45	51,54,55,56	0
3	4WL	B	360	11/11	0.94	0.09	29,32,36,36	0
3	4WL	A	360	11/11	0.94	0.10	23,26,29,31	0

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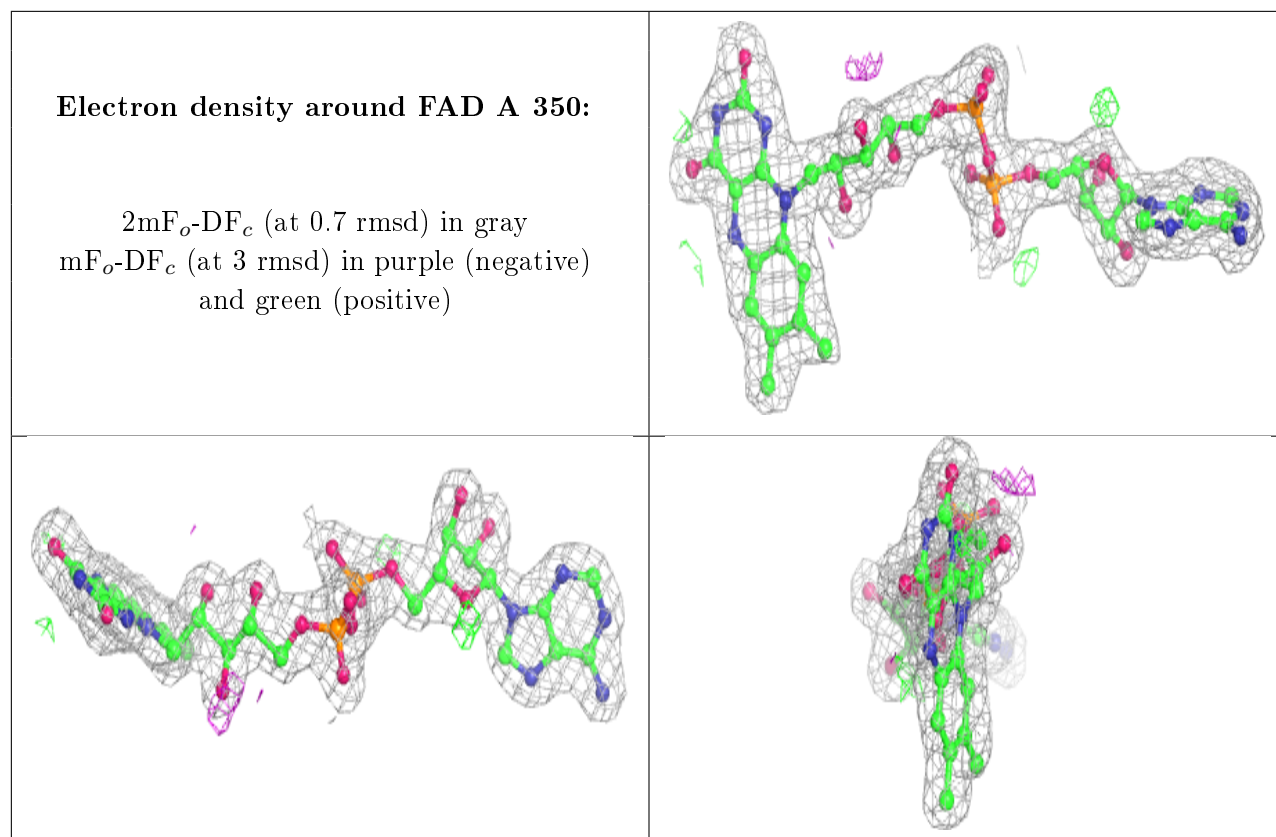
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	B	350	53/53	0.97	0.08	26,31,36,38	0
2	FAD	A	350	53/53	0.98	0.09	23,27,29,33	0

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.