



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:29 pm BST

PDB ID : 3ZNP
Title : IN VITRO AND IN VIVO INHIBITION OF HUMAN D-AMINO ACID OXIDASE: REGULATION OF D-SERINE CONCENTRATION IN THE BRAIN
Authors : Hopkins, S.C.; Heffernan, M.L.R.; Saraswat, L.D.; Bowen, C.A.; Melnick, L.; Hardy, L.W.; Orsini, M.A.; Allen, M.S.; Koch, P.; Spear, K.L.; Foglesong, R.J.; Soukri, M.; Chytil, M.; Fang, Q.K.; Jones, S.W.; Varney, M.A.; Panatier, A.; Olier, S.H.R.; Pollegioni, L.; Piubelli, L.; Molla, G.; Nardini, M.; Large, T.H.
Deposited on : 2013-02-15
Resolution : 2.40 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

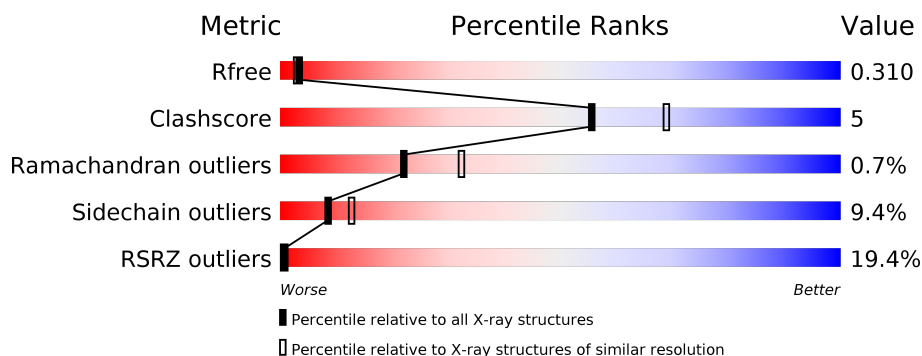
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	347	<div> <div>10%</div> <div>81%</div> <div>15%</div> <div>• •</div> </div>
1	B	347	<div> <div>28%</div> <div>77%</div> <div>19%</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
3	SE2	A	360	-	-	X	-
4	GOL	A	1343	-	-	-	X
4	GOL	B	1341	-	-	-	X
4	GOL	B	1343	-	-	-	X

2 Entry composition ⓘ

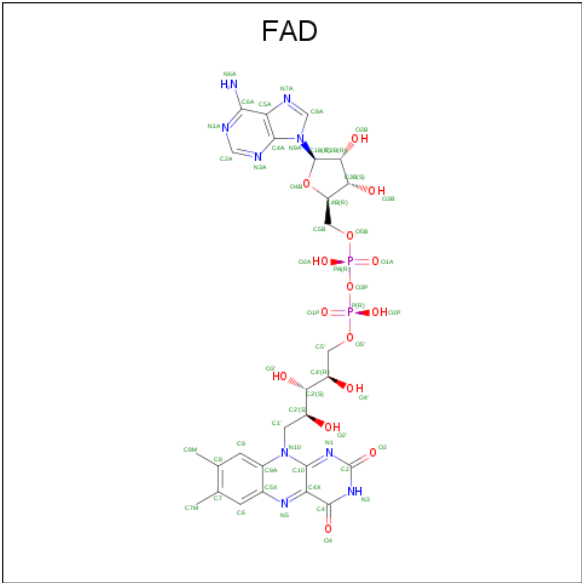
There are 5 unique types of molecules in this entry. The entry contains 5815 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

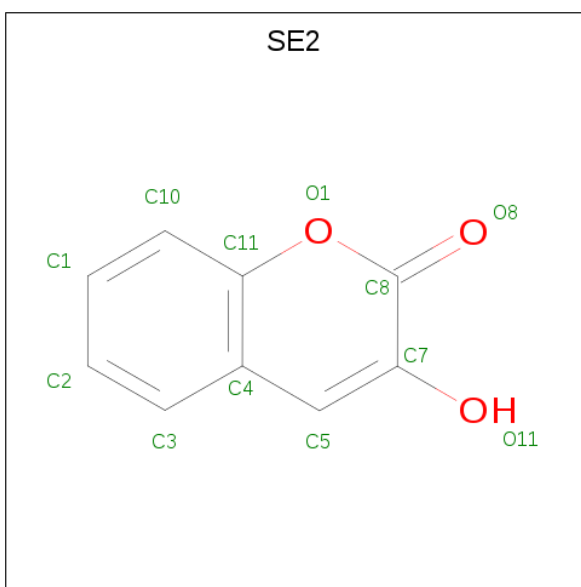
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	7	0
			2786	1787	495	495	9			
1	B	340	Total	C	N	O	S	0	3	0
			2754	1766	485	494	9			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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 3-HYDROXY-2H-CHROMEN-2-ONE (three-letter code: SE2) (formula: C₉H₆O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	9	3		

- 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	1
			12	6	6		
4	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

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

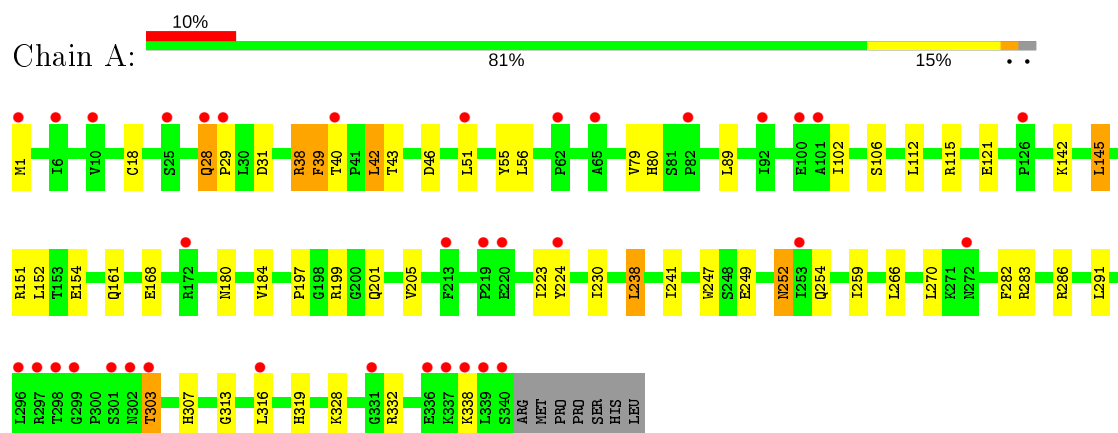
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total 79	O 79	0	9
5	B	29	Total 30	O 30	0	1

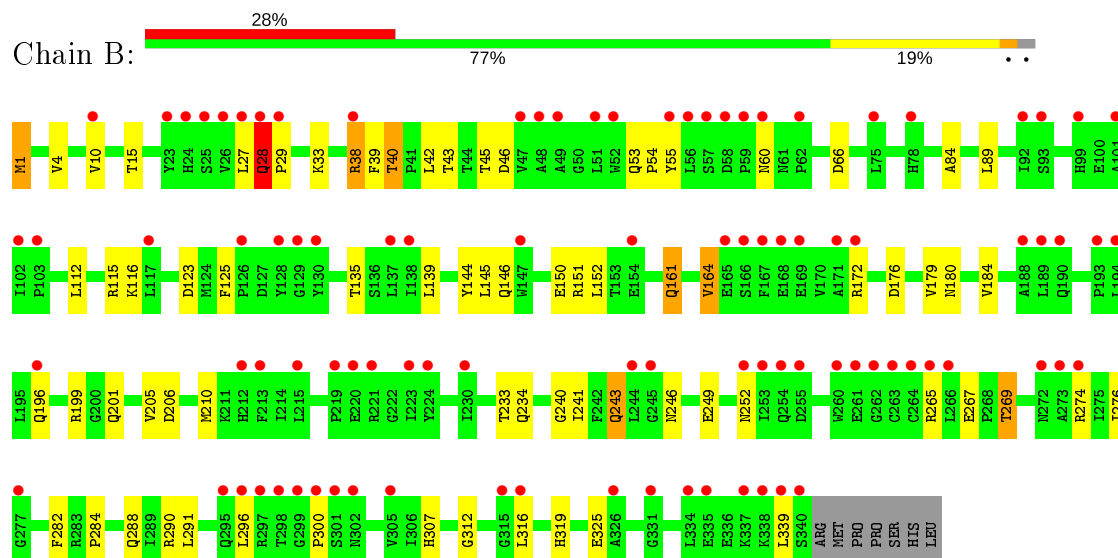
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	84.07Å 84.07Å 189.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.98 – 2.40 34.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (34.98-2.40) 98.2 (34.98-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.232 , 0.307 0.233 , 0.310	Depositor DCC
R_{free} test set	1539 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 72.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5815	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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: GOL, SE2, FAD

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	0.51	0/2882	0.78	4/3917 (0.1%)
1	B	0.48	0/2840	0.73	0/3863
All	All	0.50	0/5722	0.76	4/7780 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	THR	N-CA-C	9.68	137.15	111.00
1	A	39	PHE	C-N-CA	6.90	138.95	121.70
1	A	39	PHE	CB-CA-C	6.67	123.75	110.40
1	A	303	THR	CB-CA-C	-5.17	97.64	111.60

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	2786	0	2762	29	0
1	B	2754	0	2717	33	0
2	A	53	0	31	1	0
2	B	53	0	31	2	0
3	A	12	0	5	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	30	0	40	0	0
4	B	18	0	24	0	0
5	A	79	0	0	0	0
5	B	30	0	0	0	0
All	All	5815	0	5610	58	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (58) 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:303:THR:O	1:A:303:THR:HG22	1.74	0.87
1:A:180:ASN:HD22	1:A:307:HIS:HD2	1.25	0.82
1:A:39:PHE:O	1:A:43:THR:HG23	1.81	0.81
1:A:51:LEU:HD23	3:A:360:SE2:H1	1.66	0.78
1:B:28:GLN:HB2	1:B:29:PRO:HD3	1.74	0.69
1:A:313:GLY:O	3:A:360:SE2:H5	1.93	0.67
1:A:38[A]:ARG:HG2	2:A:350:FAD:O2B	1.95	0.64
1:A:79:VAL:HG13	1:A:80:HIS:HD2	1.64	0.63
1:A:161:GLN:HE21	1:B:249:GLU:H	1.46	0.63
1:A:316:LEU:O	1:A:319:HIS:HD2	1.82	0.63
1:A:230:ILE:HD11	3:A:360:SE2:H10	1.81	0.62
1:B:164:VAL:HG23	2:B:350:FAD:N1A	2.15	0.61
1:A:28:GLN:HG2	1:A:29:PRO:HD3	1.84	0.60
1:A:40:THR:O	1:A:46:ASP:OD1	2.20	0.59
1:A:201:GLN:HE22	1:A:252:ASN:H	1.50	0.59
1:B:233:THR:HG23	1:B:234:GLN:HG2	1.85	0.58
1:B:201:GLN:HE22	1:B:252:ASN:H	1.51	0.58
1:A:180:ASN:HD22	1:A:307:HIS:CD2	2.15	0.57
1:B:206:ASP:HB3	1:B:274:ARG:HG3	1.87	0.57
1:A:328:LYS:HE2	1:A:332:ARG:HH12	1.70	0.56
1:B:15:THR:HG21	1:B:179:VAL:HG11	1.87	0.56
1:B:112:LEU:HB2	1:B:135:THR:HB	1.89	0.55
1:B:199:ARG:HH22	1:B:201:GLN:HE21	1.54	0.54
1:B:199:ARG:HH22	1:B:201:GLN:NE2	2.07	0.52
1:B:316:LEU:O	1:B:319:HIS:HD2	1.93	0.52
1:A:199:ARG:HH22	1:A:201:GLN:HE21	1.59	0.51
1:B:40:THR:O	1:B:46:ASP:OD1	2.29	0.51
1:A:241:ILE:HD13	1:A:259:ILE:HG13	1.93	0.50
1:B:243:GLN:HE21	1:B:246:ASN:HD22	1.60	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:GLU:H	1:B:161:GLN:HE21	1.60	0.50
1:A:55:TYR:HE1	1:A:224:TYR:HH	1.59	0.49
1:B:284:PRO:HD2	1:B:312:GLY:O	2.13	0.49
1:A:161:GLN:NE2	1:B:249:GLU:H	2.11	0.48
1:B:267:GLU:HG3	1:B:269:THR:HG23	1.96	0.48
1:A:115:ARG:NH2	1:A:121:GLU:OE2	2.46	0.48
1:B:291:LEU:HD21	1:B:325:GLU:HB3	1.96	0.48
1:A:184:VAL:HG11	1:A:282:PHE:HB2	1.95	0.48
1:A:283:ARG:NE	3:A:360:SE2:O11	2.33	0.48
1:B:38[A]:ARG:HG2	2:B:350:FAD:O2B	2.15	0.47
1:B:39:PHE:O	1:B:43:THR:HG23	2.16	0.46
1:A:40:THR:HG23	1:A:145:LEU:HB3	1.97	0.45
1:B:1:MET:HA	1:B:176:ASP:OD2	2.16	0.45
1:B:144:TYR:OH	1:B:319:HIS:CE1	2.70	0.45
1:B:144:TYR:OH	1:B:319:HIS:HE1	1.99	0.45
1:A:197:PRO:HG3	1:A:247:TRP:CE2	2.52	0.44
1:B:10:VAL:HB	1:B:45:THR:HG21	1.98	0.44
1:B:139:LEU:HD11	1:B:144:TYR:CD1	2.53	0.43
1:B:53:GLN:HA	1:B:54:PRO:HD3	1.89	0.43
1:B:4:VAL:HG22	1:B:33:LYS:HB2	2.01	0.43
1:B:180:ASN:HB3	1:B:307:HIS:HA	2.02	0.42
1:B:184:VAL:HG11	1:B:282:PHE:HB2	2.00	0.42
1:A:180:ASN:ND2	1:A:307:HIS:HD2	2.04	0.42
1:B:146:GLN:HE21	1:B:150:GLU:HG3	1.84	0.42
1:A:291:LEU:HA	1:A:307:HIS:O	2.20	0.41
1:B:201:GLN:NE2	1:B:252:ASN:H	2.16	0.41
1:A:42:LEU:HD22	1:B:42:LEU:HD23	2.03	0.41
1:B:180:ASN:HD22	1:B:307:HIS:HD2	1.69	0.40
1:A:238:LEU:HD11	1:A:270:LEU:HD21	2.03	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	345/347 (99%)	324 (94%)	21 (6%)	0	100	100
1	B	341/347 (98%)	306 (90%)	30 (9%)	5 (2%)	10	14
All	All	686/694 (99%)	630 (92%)	51 (7%)	5 (1%)	22	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	300	PRO
1	B	40	THR
1	B	28	GLN
1	B	84	ALA
1	B	240	GLY

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	299/299 (100%)	273 (91%)	26 (9%)	10	15
1	B	295/299 (99%)	264 (90%)	31 (10%)	7	9
All	All	594/598 (99%)	537 (90%)	57 (10%)	8	12

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	18	CYS
1	A	28	GLN
1	A	31	ASP
1	A	38[A]	ARG
1	A	38[B]	ARG
1	A	42	LEU
1	A	56	LEU
1	A	89	LEU
1	A	102	ILE
1	A	106	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	112	LEU
1	A	142	LYS
1	A	145	LEU
1	A	151	ARG
1	A	152	LEU
1	A	154	GLU
1	A	168	GLU
1	A	205	VAL
1	A	223	ILE
1	A	238	LEU
1	A	252	ASN
1	A	254	GLN
1	A	266	LEU
1	A	286	ARG
1	A	338	LYS
1	B	1	MET
1	B	27	LEU
1	B	28	GLN
1	B	38[A]	ARG
1	B	38[B]	ARG
1	B	55	TYR
1	B	60	ASN
1	B	66	ASP
1	B	89	LEU
1	B	115	ARG
1	B	116	LYS
1	B	123	ASP
1	B	125	PHE
1	B	145	LEU
1	B	151	ARG
1	B	152	LEU
1	B	161	GLN
1	B	164	VAL
1	B	172	ARG
1	B	196	GLN
1	B	205	VAL
1	B	210	MET
1	B	241	ILE
1	B	243	GLN
1	B	265	ARG
1	B	269	THR
1	B	276	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	288	GLN
1	B	290	ARG
1	B	296	LEU
1	B	339	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	161	GLN
1	A	201	GLN
1	A	243	GLN
1	A	252	ASN
1	A	307	HIS
1	A	319	HIS
1	B	28	GLN
1	B	53	GLN
1	B	80	HIS
1	B	96	ASN
1	B	146	GLN
1	B	161	GLN
1	B	180	ASN
1	B	196	GLN
1	B	201	GLN
1	B	243	GLN
1	B	252	ASN
1	B	307	HIS
1	B	319	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

11 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	1342[B]	-	5,5,5	0.41	0	5,5,5	0.25	0
4	GOL	B	1341	-	5,5,5	0.70	0	5,5,5	0.55	0
4	GOL	A	1341	-	5,5,5	0.71	0	5,5,5	0.66	0
2	FAD	B	350	-	51,58,58	3.67	16 (31%)	60,89,89	2.63	24 (40%)
4	GOL	B	1342	-	5,5,5	0.62	0	5,5,5	0.51	0
4	GOL	B	1343	-	5,5,5	0.65	0	5,5,5	0.51	0
4	GOL	A	1344	-	5,5,5	0.58	0	5,5,5	0.56	0
4	GOL	A	1343	-	5,5,5	0.85	0	5,5,5	0.67	0
2	FAD	A	350	-	51,58,58	3.47	20 (39%)	60,89,89	2.97	24 (40%)
3	SE2	A	360	-	8,13,13	1.21	1 (12%)	10,18,18	1.05	1 (10%)
4	GOL	A	1342[A]	-	5,5,5	0.39	0	5,5,5	0.23	0

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	1342[B]	-	-	2/4/4/4	-
4	GOL	B	1341	-	-	1/4/4/4	-
4	GOL	A	1341	-	-	2/4/4/4	-
2	FAD	B	350	-	-	6/30/50/50	0/6/6/6
4	GOL	B	1342	-	-	3/4/4/4	-
4	GOL	B	1343	-	-	2/4/4/4	-
4	GOL	A	1344	-	-	4/4/4/4	-
4	GOL	A	1343	-	-	4/4/4/4	-
2	FAD	A	350	-	-	2/30/50/50	0/6/6/6
3	SE2	A	360	-	-	-	0/2/2/2
4	GOL	A	1342[A]	-	-	2/4/4/4	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	350	FAD	C4X-C10	18.63	1.57	1.38
2	A	350	FAD	C4X-C10	16.34	1.55	1.38
2	B	350	FAD	C9A-N10	11.04	1.53	1.38
2	A	350	FAD	C9A-N10	9.23	1.51	1.38
2	A	350	FAD	C10-N1	6.09	1.41	1.33
2	B	350	FAD	C2B-C1B	-6.05	1.44	1.53
2	A	350	FAD	C4X-N5	5.21	1.40	1.33
2	B	350	FAD	C10-N1	4.95	1.39	1.33
2	A	350	FAD	P-O1P	-4.66	1.34	1.50
2	A	350	FAD	C5X-N5	4.60	1.43	1.35
2	A	350	FAD	C7M-C7	4.52	1.60	1.51
2	A	350	FAD	O4-C4	4.41	1.35	1.24
2	A	350	FAD	C2-N3	-4.35	1.29	1.38
2	B	350	FAD	C4-N3	4.20	1.40	1.33
2	B	350	FAD	C6-C5X	4.04	1.48	1.41
2	B	350	FAD	C5X-N5	3.93	1.41	1.35
2	B	350	FAD	C4X-N5	3.69	1.38	1.33
2	B	350	FAD	O4-C4	3.61	1.33	1.24
2	B	350	FAD	C9-C9A	3.40	1.47	1.40
2	A	350	FAD	C9-C9A	3.11	1.46	1.40
2	A	350	FAD	O4B-C1B	3.02	1.45	1.41
2	B	350	FAD	C2A-N3A	3.00	1.36	1.32
2	B	350	FAD	O4B-C4B	-2.96	1.38	1.45
2	B	350	FAD	C8A-N7A	2.89	1.39	1.34
2	A	350	FAD	C1'-N10	-2.85	1.45	1.48
2	A	350	FAD	C4'-C3'	2.74	1.58	1.53
2	A	350	FAD	C4-N3	2.73	1.37	1.33
2	B	350	FAD	C2-N1	2.71	1.43	1.38
2	A	350	FAD	C6-C5X	2.67	1.46	1.41
2	A	350	FAD	C8A-N7A	2.44	1.39	1.34
2	B	350	FAD	P-O1P	-2.37	1.42	1.50
2	A	350	FAD	O4B-C4B	-2.32	1.39	1.45
2	A	350	FAD	C2B-C3B	-2.29	1.47	1.53
2	A	350	FAD	O3B-C3B	-2.24	1.37	1.43
2	A	350	FAD	C3B-C4B	2.23	1.58	1.53
2	B	350	FAD	C2-N3	-2.12	1.34	1.38
3	A	360	SE2	C5-C7	2.06	1.39	1.37

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	350	FAD	N3A-C2A-N1A	-9.53	113.78	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	350	FAD	C4X-N5-C5X	7.72	124.49	116.77
2	B	350	FAD	N3A-C2A-N1A	-7.69	116.65	128.68
2	A	350	FAD	C4-C4X-C10	-7.09	115.26	119.95
2	A	350	FAD	C4X-N5-C5X	6.36	123.12	116.77
2	B	350	FAD	C4-C4X-C10	-6.26	115.81	119.95
2	A	350	FAD	C4-N3-C2	5.64	119.91	115.14
2	A	350	FAD	C4-C4X-N5	5.62	125.02	118.60
2	B	350	FAD	C4-C4X-N5	5.36	124.73	118.60
2	A	350	FAD	C4A-C5A-N7A	-5.06	104.12	109.40
2	A	350	FAD	O2P-P-O1P	4.85	136.21	112.24
2	B	350	FAD	O2P-P-O1P	4.70	135.45	112.24
2	B	350	FAD	C5X-C9A-N10	4.53	121.00	117.72
2	A	350	FAD	C4X-C10-N10	-4.18	116.01	120.30
2	A	350	FAD	C5'-C4'-C3'	-4.13	104.22	112.20
2	B	350	FAD	C4A-C5A-N7A	-4.09	105.13	109.40
2	A	350	FAD	C1'-N10-C9A	4.02	121.46	118.29
2	A	350	FAD	C6-C5X-N5	3.86	123.30	119.05
2	A	350	FAD	C5X-C9A-N10	3.84	120.50	117.72
2	A	350	FAD	O5B-C5B-C4B	-3.82	95.84	108.99
2	B	350	FAD	C4X-C10-N10	-3.80	116.39	120.30
2	B	350	FAD	O5'-C5'-C4'	-3.60	99.76	109.36
2	B	350	FAD	O5B-C5B-C4B	-3.43	97.20	108.99
2	A	350	FAD	O4'-C4'-C5'	-3.38	102.32	109.92
2	B	350	FAD	C6-C5X-N5	3.37	122.76	119.05
2	A	350	FAD	C5A-C6A-N6A	3.35	125.44	120.35
2	B	350	FAD	C9A-C5X-N5	-3.15	117.43	122.36
2	A	350	FAD	C3B-C2B-C1B	-3.14	96.25	100.98
2	A	350	FAD	C2A-N1A-C6A	3.07	124.00	118.75
2	A	350	FAD	C1'-N10-C10	-3.05	115.68	118.41
2	A	350	FAD	C9A-C5X-N5	-2.94	117.77	122.36
2	A	350	FAD	C9-C9A-C5X	-2.83	115.04	119.88
2	A	350	FAD	O3'-C3'-C2'	2.76	115.47	108.81
2	B	350	FAD	C1'-N10-C9A	2.73	120.44	118.29
2	B	350	FAD	C3B-C2B-C1B	-2.71	96.90	100.98
2	B	350	FAD	C4-N3-C2	2.63	117.36	115.14
2	B	350	FAD	C10-C4X-N5	-2.61	119.46	121.26
2	B	350	FAD	O3'-C3'-C2'	2.50	114.86	108.81
2	B	350	FAD	O3B-C3B-C4B	-2.45	103.95	111.05
2	B	350	FAD	C5'-C4'-C3'	-2.44	107.49	112.20
2	A	350	FAD	C2B-C3B-C4B	2.32	107.15	102.64
2	B	350	FAD	O2P-P-O5'	-2.32	96.97	107.75
2	B	350	FAD	C9-C9A-C5X	-2.30	115.95	119.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	350	FAD	C1B-N9A-C4A	-2.24	122.70	126.64
3	A	360	SE2	C3-C4-C11	2.24	119.20	116.61
2	A	350	FAD	C10-C4X-N5	-2.22	119.72	121.26
2	B	350	FAD	C5A-C6A-N6A	2.16	123.63	120.35
2	A	350	FAD	O3B-C3B-C4B	-2.10	104.96	111.05
2	B	350	FAD	C2A-N1A-C6A	2.10	122.35	118.75

There are no chirality outliers.

All (28) torsion outliers are listed below:

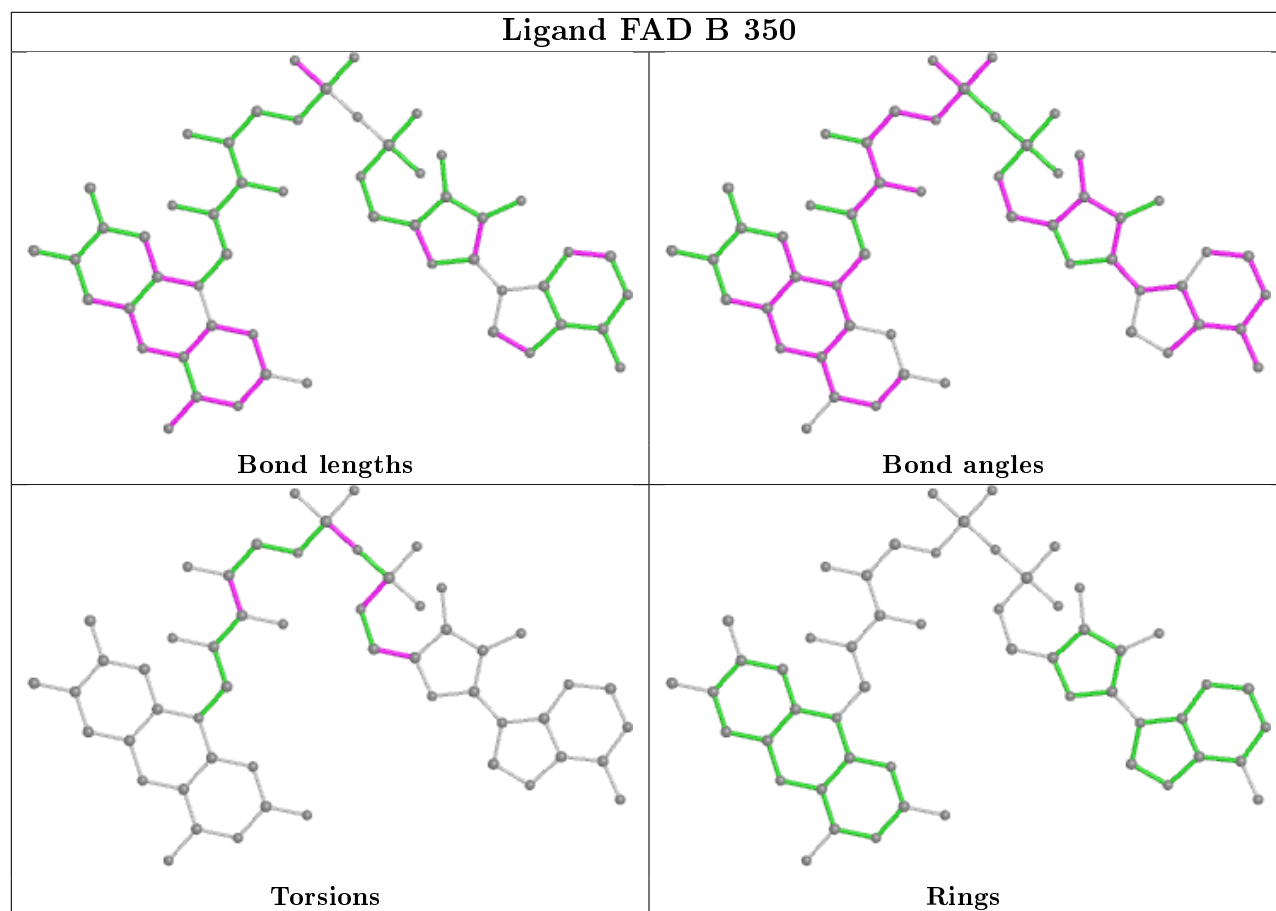
Mol	Chain	Res	Type	Atoms
4	A	1341	GOL	C1-C2-C3-O3
4	A	1343	GOL	C1-C2-C3-O3
4	A	1342[A]	GOL	C1-C2-C3-O3
2	B	350	FAD	O4B-C4B-C5B-O5B
4	B	1342	GOL	O2-C2-C3-O3
4	A	1343	GOL	O2-C2-C3-O3
2	B	350	FAD	C3B-C4B-C5B-O5B
4	A	1342[B]	GOL	C1-C2-C3-O3
4	B	1342	GOL	O1-C1-C2-C3
4	B	1342	GOL	C1-C2-C3-O3
4	A	1344	GOL	O1-C1-C2-C3
4	A	1344	GOL	C1-C2-C3-O3
4	A	1343	GOL	O1-C1-C2-C3
4	A	1342[B]	GOL	O2-C2-C3-O3
4	A	1344	GOL	O1-C1-C2-O2
4	A	1344	GOL	O2-C2-C3-O3
4	A	1342[A]	GOL	O2-C2-C3-O3
4	A	1341	GOL	O2-C2-C3-O3
4	B	1341	GOL	O2-C2-C3-O3
4	B	1343	GOL	O2-C2-C3-O3
2	A	350	FAD	C2'-C3'-C4'-C5'
2	B	350	FAD	C2'-C3'-C4'-O4'
2	B	350	FAD	C2'-C3'-C4'-C5'
2	A	350	FAD	O4B-C4B-C5B-O5B
2	B	350	FAD	PA-O3P-P-O1P
4	B	1343	GOL	C1-C2-C3-O3
2	B	350	FAD	C5B-O5B-PA-O1A
4	A	1343	GOL	O1-C1-C2-O2

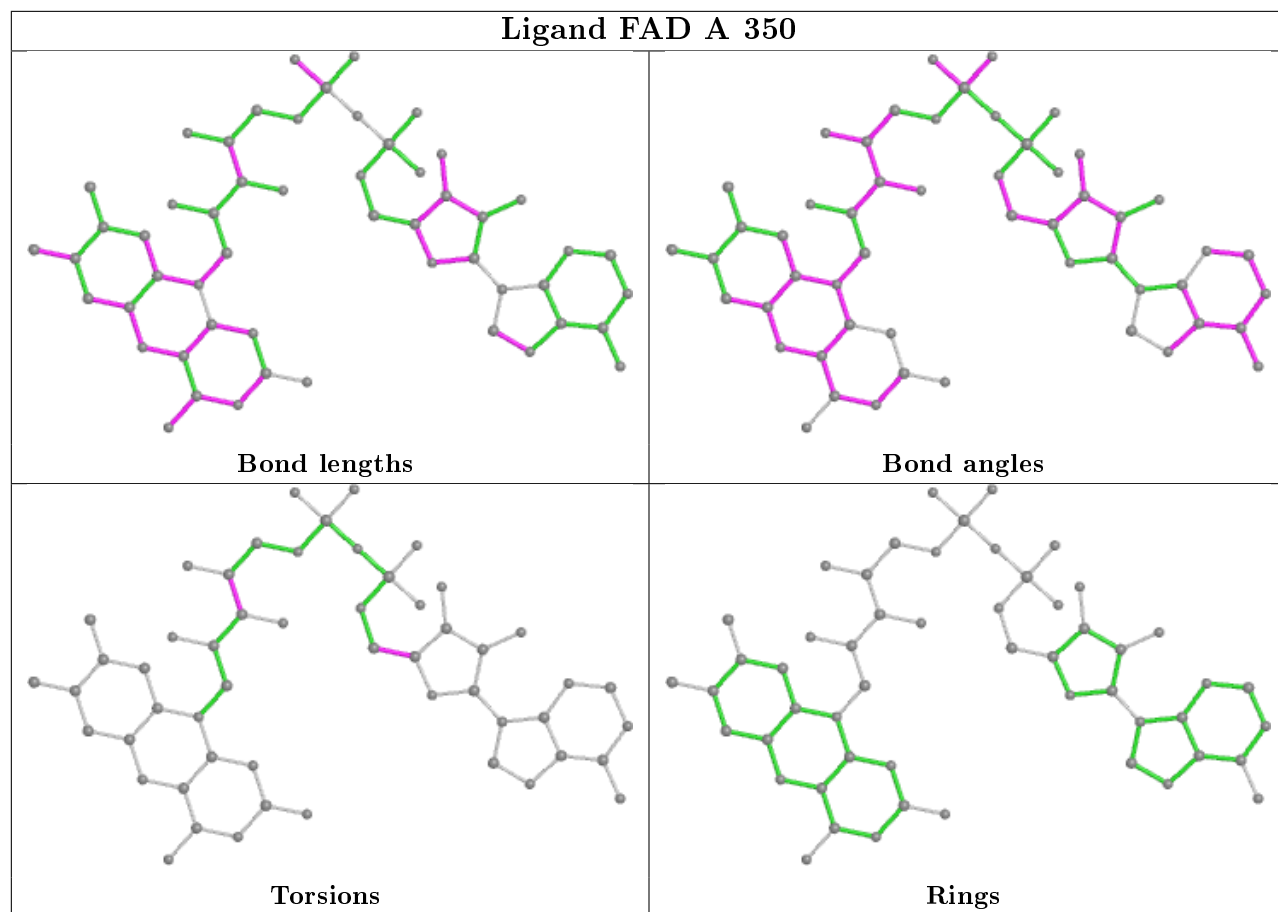
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	350	FAD	2	0
2	A	350	FAD	1	0
3	A	360	SE2	4	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	340/347 (97%)	0.63	36 (10%) 6 5	31, 67, 140, 189	0
1	B	340/347 (97%)	1.52	96 (28%) 0 0	64, 96, 151, 192	0
All	All	680/694 (97%)	1.08	132 (19%) 1 0	31, 84, 148, 192	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	ARG	8.9
1	B	298	THR	8.9
1	B	26	VAL	7.6
1	B	299	GLY	7.1
1	B	25	SER	6.9
1	B	340	SER	6.8
1	B	253	ILE	6.8
1	B	339	LEU	6.7
1	B	56	LEU	6.7
1	B	223	ILE	6.5
1	A	298	THR	6.4
1	B	57	SER	6.0
1	A	303	THR	5.9
1	B	297	ARG	5.8
1	B	219	PRO	5.7
1	B	55	TYR	5.6
1	B	194	LEU	5.5
1	B	300	PRO	5.1
1	B	338	LYS	4.8
1	B	128	TYR	4.8
1	B	60	ASN	4.8
1	B	255	ASP	4.7
1	A	301	SER	4.6
1	B	126	PRO	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	221	ARG	4.5
1	B	51	LEU	4.4
1	A	339	LEU	4.4
1	B	167	PHE	4.4
1	B	168	GLU	4.3
1	B	261	GLU	4.3
1	B	129	GLY	4.2
1	B	24	HIS	4.1
1	B	302	ASN	4.1
1	B	102	ILE	4.0
1	B	117	LEU	3.9
1	A	302	ASN	3.9
1	B	245	GLY	3.9
1	B	92	ILE	3.8
1	A	220	GLU	3.8
1	B	29	PRO	3.8
1	B	193	PRO	3.8
1	B	273	ALA	3.7
1	B	188	ALA	3.7
1	B	316	LEU	3.7
1	B	230	ILE	3.7
1	B	137	LEU	3.7
1	B	49	ALA	3.7
1	B	103	PRO	3.7
1	B	274	ARG	3.6
1	A	29	PRO	3.6
1	B	295	GLN	3.6
1	A	338	LYS	3.6
1	B	138[A]	ILE	3.5
1	A	337	LYS	3.5
1	B	172	ARG	3.5
1	B	337	LYS	3.4
1	B	166	SER	3.3
1	A	62	PRO	3.3
1	B	48	ALA	3.3
1	A	65	ALA	3.2
1	B	28	GLN	3.2
1	B	331	GLY	3.2
1	B	190	GLN	3.2
1	B	189	LEU	3.2
1	A	126	PRO	3.2
1	B	165	GLU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	254	GLN	3.0
1	B	244	LEU	3.0
1	B	169	GLU	2.9
1	A	100	GLU	2.9
1	A	336	GLU	2.9
1	B	212	HIS	2.9
1	B	263	CYS	2.9
1	B	220	GLU	2.9
1	A	40	THR	2.8
1	A	253	ILE	2.8
1	B	27	LEU	2.8
1	B	296	LEU	2.8
1	B	38[A]	ARG	2.7
1	A	316	LEU	2.7
1	B	266	LEU	2.7
1	B	272	ASN	2.7
1	B	262	GLY	2.6
1	B	264	CYS	2.6
1	B	265	ARG	2.6
1	A	25	SER	2.6
1	A	296	LEU	2.6
1	B	260	TRP	2.6
1	B	101	ALA	2.5
1	A	172[A]	ARG	2.5
1	B	52	TRP	2.5
1	B	10	VAL	2.4
1	B	305	VAL	2.4
1	A	272	ASN	2.4
1	B	315	GLY	2.4
1	B	147	TRP	2.4
1	B	252	ASN	2.4
1	A	219	PRO	2.3
1	A	51	LEU	2.3
1	B	196	GLN	2.3
1	A	28	GLN	2.3
1	A	1	MET	2.3
1	B	326	ALA	2.3
1	B	78	HIS	2.3
1	A	299	GLY	2.3
1	B	130	TYR	2.3
1	B	224	TYR	2.3
1	A	331	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	82	PRO	2.2
1	A	10	VAL	2.2
1	B	215	LEU	2.2
1	A	340	SER	2.2
1	B	301	SER	2.2
1	A	6	ILE	2.2
1	B	213	PHE	2.2
1	B	58	ASP	2.2
1	A	224	TYR	2.1
1	B	23	TYR	2.1
1	B	171	ALA	2.1
1	B	334	LEU	2.1
1	A	213	PHE	2.1
1	B	99	HIS	2.1
1	B	154	GLU	2.1
1	A	101	ALA	2.1
1	B	335	GLU	2.1
1	B	59	PRO	2.1
1	B	93	SER	2.0
1	B	277	GLY	2.0
1	B	75	LEU	2.0
1	B	62	PRO	2.0
1	B	47	VAL	2.0
1	A	92	ILE	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](#)

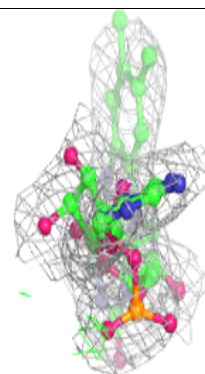
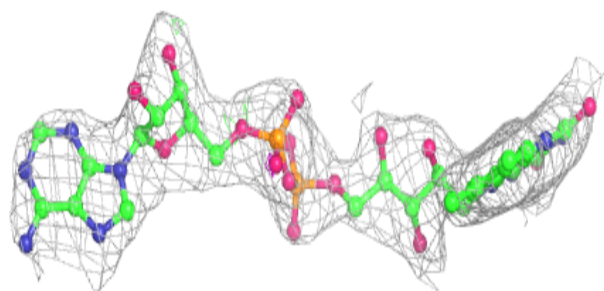
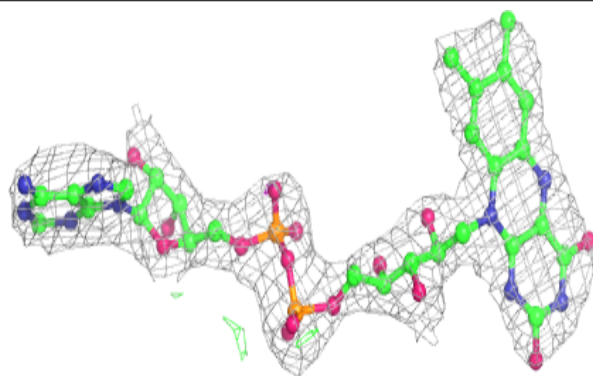
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

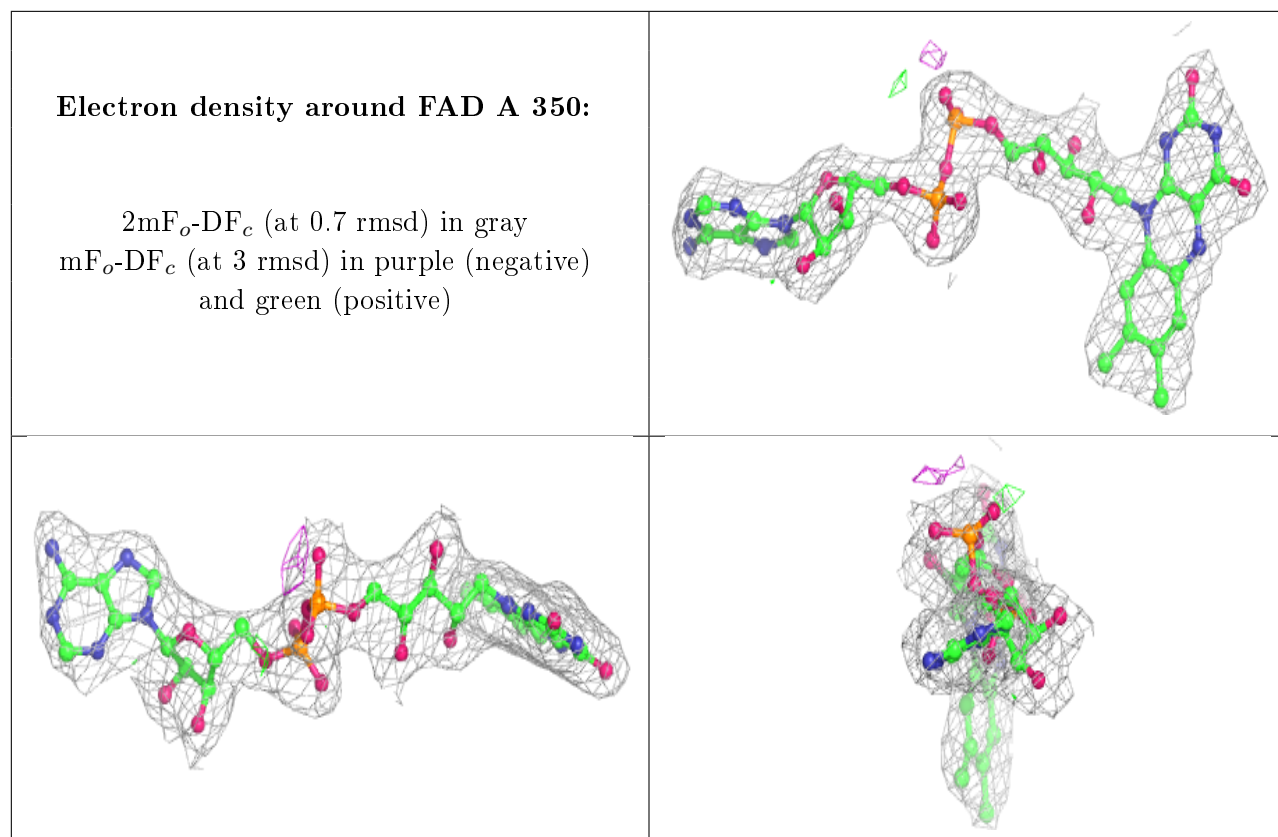
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	B	1343	6/6	0.20	0.46	116,117,117,118	0
4	GOL	B	1342	6/6	0.31	0.31	121,122,122,122	0
4	GOL	A	1343	6/6	0.38	0.55	102,104,104,104	0
4	GOL	B	1341	6/6	0.51	0.45	119,120,120,121	0
4	GOL	A	1344	6/6	0.75	0.24	96,98,98,98	0
4	GOL	A	1342[B]	6/6	0.78	0.28	103,104,104,105	6
4	GOL	A	1342[A]	6/6	0.78	0.28	99,99,99,100	6
4	GOL	A	1341	6/6	0.85	0.44	100,102,102,102	0
2	FAD	B	350	53/53	0.88	0.19	65,72,78,81	0
3	SE2	A	360	12/12	0.91	0.19	59,67,72,73	0
2	FAD	A	350	53/53	0.97	0.18	32,44,61,67	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 FAD B 350:

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.