



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 06:33 PM UTC

PDB ID : 1QLU / pdb_00001qlu
Title : STRUCTURE OF THE H422A MUTANT VANILLYL-ALCOHOL OXIDASE
IN COMPLEX WITH ISOEUGENOL
Authors : Mattevi, A.
Deposited on : 1999-09-16
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 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	:	FAILED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

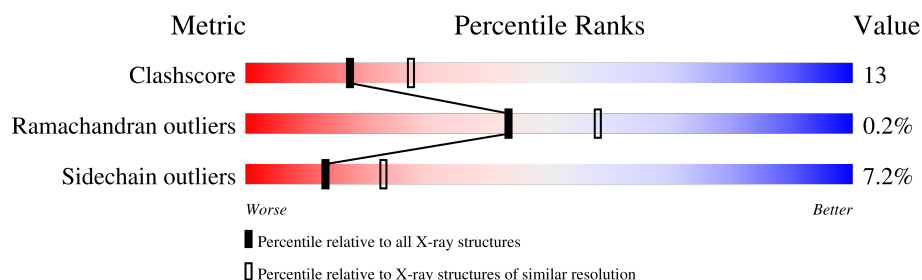
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	560	 66% 24% 7% . .
1	B	560	 60% 30% 6% . .

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 9076 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 VANILLYL-ALCOHOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	66	0	0
			4346	2790	742	790	24			
1	B	550	Total	C	N	O	S	66	0	0
			4346	2790	742	790	24			

There are 4 discrepancies between the modelled and reference sequences:

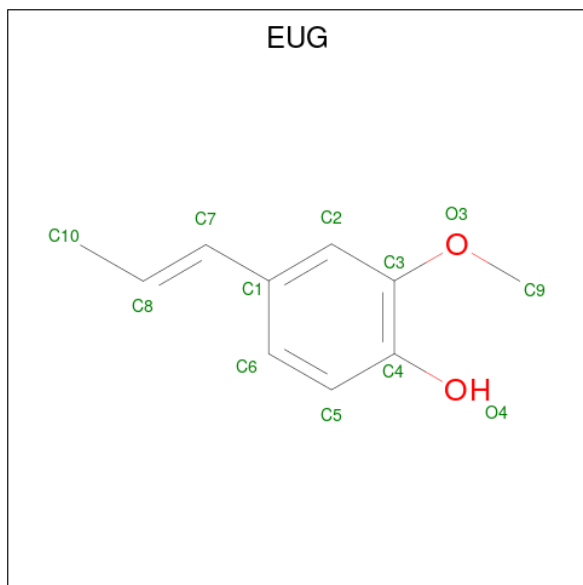
Chain	Residue	Modelled	Actual	Comment	Reference
A	274	GLY	ARG	conflict	UNP P56216
A	422	ALA	HIS	engineered mutation	UNP P56216
B	274	GLY	ARG	conflict	UNP P56216
B	422	ALA	HIS	engineered mutation	UNP P56216

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: 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		

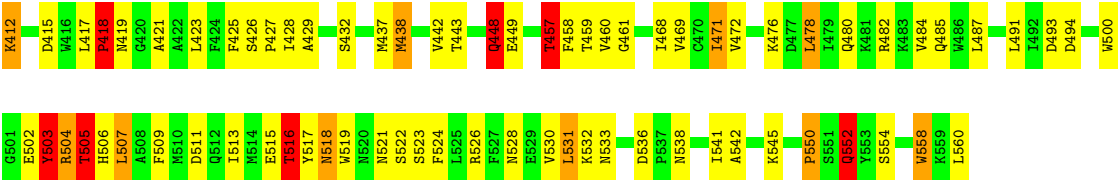
- Molecule 3 is 2-methoxy-4-[(1E)-prop-1-en-1-yl]phenol (CCD ID: EUG) (formula: C₁₀H₁₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	9	2		
3	B	1	Total	C	O	0	0
			11	9	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	139	Total	O	0	0
			139	139		
4	B	117	Total	O	0	0
			117	117		



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	129.84Å 129.84Å 133.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40	Depositor
% Data completeness (in resolution range)	94.8 (30.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.219 , 0.273	Depositor
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.488	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.006 for l,-k,h 0.023 for -l,-k,-h 0.022 for -h,-l,-k 0.006 for -h,l,k 0.040 for -h,k,-l	Xtriage
Total number of atoms	9076	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.99	3/4464 (0.1%)	2.02	117/6067 (1.9%)
1	B	1.01	5/4464 (0.1%)	2.07	146/6067 (2.4%)
All	All	1.00	8/8928 (0.1%)	2.04	263/12134 (2.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	52	MET	CB-CG	34.34	2.55	1.52
1	A	52	MET	CB-CG	32.80	2.50	1.52
1	B	350	ARG	CZ-NH1	10.73	1.47	1.32
1	A	350	ARG	CZ-NH1	10.45	1.47	1.32
1	B	372	LYS	CD-CE	-6.52	1.32	1.52
1	B	266	GLY	CA-C	6.28	1.56	1.52
1	A	372	LYS	CD-CE	-5.38	1.36	1.52
1	B	350	ARG	CZ-NH2	-5.17	1.26	1.33

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	350	ARG	NE-CZ-NH1	-29.93	91.57	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	350	ARG	NE-CZ-NH1	-29.77	91.73	121.50
1	B	211	ARG	CA-CB-CG	24.26	162.62	114.10
1	B	211	ARG	CD-NE-CZ	20.84	153.58	124.40
1	A	211	ARG	CD-NE-CZ	19.40	151.56	124.40
1	A	211	ARG	CA-CB-CG	17.88	149.87	114.10
1	A	52	MET	CA-CB-CG	-15.30	83.50	114.10
1	B	52	MET	CA-CB-CG	-14.43	85.23	114.10
1	A	114	ARG	CB-CG-CD	12.87	140.90	111.30
1	B	297	ARG	CD-NE-CZ	11.63	140.68	124.40
1	A	37	VAL	CA-C-O	-11.45	107.85	120.67
1	A	7	PHE	CA-CB-CG	11.41	125.21	113.80
1	A	297	ARG	CD-NE-CZ	10.92	139.69	124.40
1	B	127	MET	CA-C-N	10.52	140.12	121.92
1	B	127	MET	C-N-CA	10.52	140.12	121.92
1	B	7	PHE	CA-CB-CG	10.34	124.14	113.80
1	A	30	ARG	CA-CB-CG	10.26	134.61	114.10
1	A	350	ARG	NE-CZ-NH2	10.17	128.35	119.20
1	A	552	GLN	CA-CB-CG	10.07	134.24	114.10
1	B	7	PHE	N-CA-C	9.98	126.41	112.04
1	B	30	ARG	CA-CB-CG	9.88	133.85	114.10
1	A	341	LYS	CA-CB-CG	9.76	133.61	114.10
1	A	127	MET	CA-C-N	9.67	138.99	122.26
1	A	127	MET	C-N-CA	9.67	138.99	122.26
1	B	350	ARG	NE-CZ-NH2	9.31	127.58	119.20
1	A	7	PHE	N-CA-C	9.30	125.43	112.04
1	B	552	GLN	CB-CG-CD	9.27	128.36	112.60
1	A	128	ASN	N-CA-C	9.25	124.75	113.38
1	B	536	ASP	CA-CB-CG	9.19	121.79	112.60
1	A	128	ASN	CB-CA-C	-9.12	93.78	109.65
1	A	221	LYS	CB-CG-CD	9.08	132.18	111.30
1	B	518	ASN	OD1-CG-ND2	-8.98	113.62	122.60
1	B	552	GLN	CA-CB-CG	8.96	132.03	114.10
1	B	515	GLU	CA-C-N	8.82	133.72	120.31
1	B	515	GLU	C-N-CA	8.82	133.72	120.31
1	B	528	ASN	CA-CB-CG	-8.80	103.80	112.60
1	B	347	ASN	CA-CB-CG	-8.79	103.81	112.60
1	A	552	GLN	OE1-CD-NE2	-8.74	113.86	122.60
1	B	53	LYS	CB-CG-CD	-8.69	91.31	111.30
1	B	221	LYS	CB-CG-CD	8.68	131.27	111.30
1	B	560	LEU	CA-C-O	-8.63	106.12	120.80
1	A	552	GLN	CB-CG-CD	8.62	127.25	112.60
1	B	24	PHE	CA-CB-CG	8.55	122.35	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	ASN	CA-CB-CG	8.52	121.12	112.60
1	B	168	VAL	N-CA-C	8.50	117.28	107.84
1	B	347	ASN	OD1-CG-ND2	8.47	131.07	122.60
1	A	153	ASN	CA-CB-CG	8.28	120.88	112.60
1	A	114	ARG	NE-CZ-NH2	-8.22	111.80	119.20
1	B	341	LYS	CA-CB-CG	8.06	130.22	114.10
1	A	347	ASN	CA-CB-CG	-7.90	104.70	112.60
1	A	104	ARG	CD-NE-CZ	7.89	135.45	124.40
1	B	153	ASN	CA-CB-CG	7.79	120.39	112.60
1	B	128	ASN	N-CA-C	7.73	123.00	113.50
1	A	129	ARG	N-CA-C	7.67	121.96	109.76
1	B	494	ASP	CA-CB-CG	7.64	120.24	112.60
1	A	528	ASN	CA-CB-CG	-7.63	104.97	112.60
1	A	560	LEU	CA-C-O	-7.63	107.83	120.80
1	A	142	VAL	N-CA-CB	-7.60	98.29	112.36
1	B	128	ASN	CB-CA-C	-7.57	95.52	109.29
1	A	168	VAL	N-CA-C	7.56	116.23	107.84
1	A	526	ARG	CD-NE-CZ	7.54	134.95	124.40
1	B	482	ARG	CD-NE-CZ	7.53	134.94	124.40
1	B	457	THR	CB-CA-C	-7.51	92.89	109.56
1	B	558	TRP	N-CA-C	7.50	122.72	112.90
1	B	129	ARG	N-CA-C	7.49	121.37	110.28
1	B	74	ILE	CA-C-N	-7.38	113.48	123.14
1	B	74	ILE	C-N-CA	-7.38	113.48	123.14
1	A	264	LYS	CA-C-O	-7.37	112.79	120.89
1	B	505	THR	CB-CA-C	-7.33	94.50	111.95
1	A	509	PHE	CA-CB-CG	-7.26	106.54	113.80
1	A	426	SER	N-CA-C	7.13	121.94	108.97
1	A	457	THR	CB-CA-C	-7.08	93.85	109.56
1	B	524	PHE	CA-C-O	-7.07	113.40	120.82
1	A	240	HIS	CA-CB-CG	-7.05	106.75	113.80
1	B	242	PHE	CA-C-O	-7.04	114.10	119.59
1	B	509	PHE	CA-CB-CG	-7.00	106.80	113.80
1	A	128	ASN	N-CA-CB	-7.00	100.11	110.53
1	B	493	ASP	CA-C-O	-6.91	113.74	121.00
1	B	67	ASP	CA-CB-CG	6.91	119.51	112.60
1	A	558	TRP	N-CA-C	6.88	121.91	112.90
1	B	423	LEU	CA-C-O	-6.83	111.87	120.28
1	A	482	ARG	CD-NE-CZ	6.83	133.96	124.40
1	B	104	ARG	CD-NE-CZ	6.83	133.96	124.40
1	B	531	LEU	O-C-N	6.79	129.06	122.07
1	A	549	TRP	O-C-N	6.78	127.42	121.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	GLY	O-C-N	-6.77	118.74	123.95
1	A	330	ARG	NE-CZ-NH2	6.76	125.29	119.20
1	B	506	HIS	N-CA-CB	-6.76	100.18	110.45
1	B	142	VAL	N-CA-CB	-6.75	99.86	112.36
1	B	426	SER	N-CA-C	6.75	121.26	108.97
1	B	105	ASN	OD1-CG-ND2	-6.74	115.86	122.60
1	A	217	LEU	CB-CA-C	6.72	117.81	110.08
1	A	53	LYS	CB-CG-CD	-6.70	95.88	111.30
1	B	504	ARG	NE-CZ-NH2	-6.70	113.17	119.20
1	B	285	LYS	N-CA-C	6.67	120.91	110.17
1	A	505	THR	CB-CA-C	-6.63	96.05	111.09
1	A	211	ARG	CB-CG-CD	6.61	126.51	111.30
1	B	458	PHE	CA-CB-CG	6.51	120.31	113.80
1	B	409	ASP	CA-CB-CG	-6.49	106.11	112.60
1	B	71	ALA	CA-C-O	-6.48	114.35	121.87
1	B	425	PHE	CA-C-N	-6.45	115.02	123.34
1	B	425	PHE	C-N-CA	-6.45	115.02	123.34
1	B	533	ASN	OD1-CG-ND2	-6.42	116.18	122.60
1	B	211	ARG	NE-CZ-NH2	6.40	124.96	119.20
1	A	424	PHE	N-CA-C	6.33	119.04	108.73
1	B	523	SER	CA-C-N	6.32	128.66	120.44
1	B	523	SER	C-N-CA	6.32	128.66	120.44
1	B	114	ARG	CB-CG-CD	6.30	125.79	111.30
1	B	168	VAL	CB-CA-C	-6.30	101.75	111.89
1	A	214	MET	CG-SD-CE	6.29	114.74	100.90
1	A	267	ILE	CA-C-O	6.28	126.61	120.27
1	A	285	LYS	N-CA-C	6.27	120.27	110.17
1	B	415	ASP	CA-CB-CG	-6.25	106.36	112.60
1	B	437	MET	CB-CA-C	-6.24	101.09	110.88
1	B	124	GLY	N-CA-C	6.24	121.73	113.37
1	A	304	ALA	N-CA-C	-6.21	104.61	111.82
1	A	185	VAL	CA-C-N	6.21	127.03	121.82
1	A	185	VAL	C-N-CA	6.21	127.03	121.82
1	B	128	ASN	N-CA-CB	-6.17	101.45	110.53
1	A	149	HIS	CB-CG-CD2	6.17	139.22	131.20
1	A	505	THR	N-CA-CB	6.16	121.29	111.56
1	A	506	HIS	N-CA-CB	-6.14	101.12	110.45
1	A	504	ARG	NE-CZ-NH2	-6.12	113.69	119.20
1	B	429	ALA	N-CA-CB	-6.12	101.29	111.20
1	A	8	ARG	CA-CB-CG	6.11	126.33	114.10
1	A	385	PHE	N-CA-C	-6.07	101.28	110.50
1	A	297	ARG	NE-CZ-NH2	-6.04	113.76	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	ARG	CB-CG-CD	6.03	125.16	111.30
1	A	67	ASP	CA-CB-CG	6.00	118.61	112.60
1	A	491	LEU	O-C-N	5.99	128.47	122.12
1	B	460	VAL	N-CA-C	5.99	117.07	107.73
1	A	24	PHE	CA-CB-CG	5.98	119.78	113.80
1	B	372	LYS	CG-CD-CE	5.98	125.06	111.30
1	A	8	ARG	CB-CG-CD	5.97	125.03	111.30
1	B	256	GLN	OE1-CD-NE2	-5.92	116.68	122.60
1	B	211	ARG	NE-CZ-NH1	-5.91	115.59	121.50
1	A	552	GLN	CA-C-N	5.90	132.49	123.23
1	A	552	GLN	C-N-CA	5.90	132.49	123.23
1	A	536	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	515	GLU	CA-C-N	5.89	128.77	120.28
1	A	515	GLU	C-N-CA	5.89	128.77	120.28
1	B	186	GLY	CA-C-O	5.88	126.82	121.47
1	B	438	MET	CA-C-O	-5.87	114.33	120.55
1	B	461	GLY	CA-C-O	-5.86	115.82	122.33
1	A	536	ASP	O-C-N	-5.85	116.04	121.36
1	A	314	ILE	N-CA-C	5.84	116.58	110.62
1	B	329	SER	CA-C-O	5.83	126.38	119.56
1	A	516	THR	N-CA-CB	-5.79	101.30	110.22
1	A	65	ASP	CA-CB-CG	5.77	118.37	112.60
1	B	448	GLN	OE1-CD-NE2	-5.75	116.85	122.60
1	B	505	THR	N-CA-CB	5.74	120.80	111.21
1	A	460	VAL	N-CA-C	5.74	116.68	107.73
1	A	74	ILE	CA-C-O	-5.74	114.40	120.48
1	A	448	GLN	OE1-CD-NE2	-5.70	116.90	122.60
1	B	532	LYS	CA-C-O	-5.70	114.51	120.55
1	B	149	HIS	N-CA-CB	5.69	118.26	110.01
1	B	246	PHE	CA-C-O	-5.67	114.81	121.44
1	B	503	TYR	CA-C-O	5.67	125.38	119.14
1	A	347	ASN	OD1-CG-ND2	5.67	128.26	122.60
1	B	330	ARG	N-CA-CB	-5.67	101.71	110.04
1	B	303	MET	N-CA-C	5.66	119.49	112.58
1	B	38	GLU	CB-CG-CD	5.66	122.22	112.60
1	B	153	ASN	OD1-CG-ND2	-5.64	116.96	122.60
1	B	187	TYR	CA-CB-CG	-5.64	103.75	113.90
1	A	336	ASP	CA-CB-CG	-5.63	106.97	112.60
1	B	55	THR	CA-C-O	-5.62	115.18	121.81
1	A	8	ARG	NE-CZ-NH2	5.62	124.25	119.20
1	B	350	ARG	CA-C-O	5.62	126.27	119.31
1	A	390	PRO	CA-C-N	5.61	129.57	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	PRO	C-N-CA	5.61	129.57	120.60
1	A	168	VAL	CB-CA-C	-5.61	102.87	111.89
1	B	221	LYS	CG-CD-CE	5.59	124.17	111.30
1	B	471	ILE	CA-C-N	-5.58	115.90	123.10
1	B	471	ILE	C-N-CA	-5.58	115.90	123.10
1	A	57	THR	CA-C-O	5.55	125.52	119.24
1	B	272	ASN	OD1-CG-ND2	5.55	128.16	122.60
1	A	145	GLY	N-CA-C	5.55	120.78	114.67
1	A	113	PRO	CA-C-O	-5.55	115.09	121.86
1	A	264	LYS	CB-CA-C	-5.55	100.01	110.16
1	B	99	PRO	CA-C-O	5.54	127.35	121.03
1	A	457	THR	N-CA-CB	5.54	121.83	111.53
1	A	471	ILE	CA-C-N	-5.53	115.90	123.14
1	A	471	ILE	C-N-CA	-5.53	115.90	123.14
1	A	124	GLY	N-CA-C	5.52	120.76	113.37
1	B	476	LYS	CA-C-O	5.52	126.10	119.59
1	B	297	ARG	CA-C-N	5.50	125.16	119.05
1	B	297	ARG	C-N-CA	5.50	125.16	119.05
1	A	313	HIS	CA-C-O	-5.50	115.57	121.56
1	B	117	GLY	N-CA-C	-5.49	107.78	114.92
1	A	437	MET	CB-CA-C	-5.48	102.28	110.88
1	B	114	ARG	N-CA-CB	5.48	118.17	110.12
1	A	405	ILE	CA-C-O	5.47	122.75	119.19
1	A	236	SER	CA-CB-OG	-5.47	100.16	111.10
1	B	304	ALA	N-CA-C	-5.43	105.38	112.23
1	A	331	THR	N-CA-C	-5.42	107.04	113.97
1	B	58	HIS	CA-CB-CG	-5.41	108.39	113.80
1	B	421	ALA	CA-C-N	-5.41	114.32	122.81
1	B	421	ALA	C-N-CA	-5.41	114.32	122.81
1	B	530	VAL	CA-C-O	-5.40	115.33	120.95
1	A	505	THR	OG1-CB-CG2	5.40	120.10	109.30
1	A	221	LYS	CG-CD-CE	5.38	123.68	111.30
1	B	264	LYS	CA-C-O	-5.37	114.97	120.99
1	B	448	GLN	CB-CG-CD	5.35	121.69	112.60
1	B	370	THR	CA-CB-OG1	-5.33	101.60	109.60
1	A	183	ARG	NE-CZ-NH1	-5.32	116.18	121.50
1	A	330	ARG	N-CA-CB	-5.32	102.22	110.04
1	B	113	PRO	CA-C-O	-5.32	115.37	121.86
1	B	296	ILE	N-CA-C	5.32	116.05	110.62
1	B	112	ALA	N-CA-C	5.32	116.39	109.64
1	B	485	GLN	CA-C-O	-5.30	114.93	120.55
1	B	37	VAL	CA-C-O	-5.29	114.74	120.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	LYS	CG-CD-CE	5.29	123.47	111.30
1	B	516	THR	CA-CB-CG2	5.28	119.48	110.50
1	A	350	ARG	NH1-CZ-NH2	-5.28	112.44	119.30
1	B	254	PHE	CA-C-N	-5.27	115.72	123.00
1	B	254	PHE	C-N-CA	-5.27	115.72	123.00
1	A	297	ARG	CA-C-N	5.26	124.89	119.05
1	A	297	ARG	C-N-CA	5.26	124.89	119.05
1	B	507	LEU	N-CA-C	5.26	117.69	111.33
1	B	114	ARG	NE-CZ-NH2	-5.25	114.47	119.20
1	B	412	LYS	CA-C-O	-5.25	114.33	120.20
1	A	187	TYR	CA-CB-CG	-5.24	104.47	113.90
1	B	198	SER	CA-C-O	-5.24	113.85	119.98
1	B	457	THR	N-CA-CB	5.22	121.25	111.53
1	A	56	HIS	CA-CB-CG	5.22	119.02	113.80
1	B	538	ASN	CA-CB-CG	-5.21	107.39	112.60
1	B	306	GLN	N-CA-C	5.21	118.09	111.69
1	B	149	HIS	CB-CG-CD2	5.20	137.96	131.20
1	B	138	ALA	O-C-N	5.20	129.10	122.86
1	B	419	ASN	OD1-CG-ND2	5.18	127.78	122.60
1	A	498	ASN	CB-CG-ND2	5.18	124.16	116.40
1	B	222	ARG	CB-CA-C	5.18	116.96	109.92
1	B	195	MET	CG-SD-CE	-5.17	89.52	100.90
1	B	72	SER	N-CA-C	-5.17	107.14	113.50
1	A	412	LYS	CA-C-O	-5.17	114.26	120.10
1	A	314	ILE	O-C-N	-5.16	116.87	121.87
1	A	491	LEU	CA-C-O	-5.15	115.09	120.55
1	A	303	MET	N-CA-C	5.15	118.86	112.58
1	B	340	ASP	CA-CB-CG	5.15	117.75	112.60
1	B	442	VAL	CA-C-N	5.14	127.17	120.28
1	B	442	VAL	C-N-CA	5.14	127.17	120.28
1	A	490	THR	CA-CB-OG1	-5.12	101.92	109.60
1	B	174	GLY	CA-C-N	5.12	129.41	122.19
1	B	174	GLY	C-N-CA	5.12	129.41	122.19
1	B	336	ASP	CA-CB-CG	-5.12	107.48	112.60
1	B	235	TRP	CA-C-O	-5.11	115.38	121.56
1	B	147	THR	CA-C-O	-5.11	115.91	121.89
1	B	528	ASN	CB-CG-ND2	5.11	124.06	116.40
1	A	15	LYS	N-CA-C	5.07	119.31	113.38
1	B	550	PRO	N-CA-C	-5.07	103.48	111.34
1	B	56	HIS	CA-CB-CG	5.07	118.87	113.80
1	A	149	HIS	CB-CG-ND1	-5.07	115.10	122.70
1	B	215	GLY	O-C-N	-5.06	117.06	122.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	ARG	CB-CG-CD	5.06	122.94	111.30
1	B	114	ARG	NE-CZ-NH1	5.05	126.55	121.50
1	A	58	HIS	CA-CB-CG	-5.04	108.76	113.80
1	A	458	PHE	CA-CB-CG	5.04	118.84	113.80
1	A	521	ASN	OD1-CG-ND2	5.02	127.62	122.60
1	A	438	MET	CA-C-O	-5.01	115.24	120.55
1	B	224	GLU	N-CA-C	5.01	118.17	111.75
1	A	79	ASN	N-CA-CB	-5.01	103.69	111.35
1	B	204	LEU	CA-C-N	5.00	127.48	120.28
1	B	204	LEU	C-N-CA	5.00	127.48	120.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	350	ARG	Sidechain
1	B	350	ARG	Sidechain

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	4346	0	4288	112	1
1	B	4346	0	4288	111	1
2	A	53	0	31	5	0
2	B	53	0	31	8	0
3	A	11	0	7	2	0
3	B	11	0	8	2	0
4	A	139	0	0	9	0
4	B	117	0	0	3	0
All	All	9076	0	8653	216	1

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 13.

All (216) 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)
2:B:600:FAD:H8A	2:B:600:FAD:C5B	1.73	1.17
2:A:600:FAD:C5B	2:A:600:FAD:H8A	1.75	1.15
2:A:600:FAD:H51A	2:A:600:FAD:C8A	1.86	1.04
2:B:600:FAD:H8A	2:B:600:FAD:H51A	1.04	1.03
1:A:349:GLY:H	1:A:352:ASN:HD21	1.09	1.00
2:B:600:FAD:H51A	2:B:600:FAD:C8A	1.90	0.99
2:A:600:FAD:H8A	2:A:600:FAD:H51A	1.00	0.97
1:B:349:GLY:H	1:B:352:ASN:HD21	1.15	0.91
1:B:550:PRO:HB2	1:B:552:GLN:NE2	1.86	0.90
1:A:550:PRO:HB2	1:A:552:GLN:NE2	1.89	0.87
1:A:189:PRO:HG2	1:A:270:MET:HE1	1.57	0.85
1:A:516:THR:HG21	4:A:2122:HOH:O	1.80	0.79
1:A:149:HIS:HD1	1:A:408:TYR:HH	1.25	0.76
1:B:189:PRO:HG2	1:B:270:MET:HE1	1.68	0.75
1:B:550:PRO:HB2	1:B:552:GLN:HE22	1.50	0.74
1:A:505:THR:HG21	1:A:513:ILE:HD12	1.68	0.73
1:A:550:PRO:HB2	1:A:552:GLN:HE22	1.53	0.72
1:B:505:THR:HG21	1:B:513:ILE:HD12	1.69	0.71
1:B:102:ILE:HG22	1:B:104:ARG:HG3	1.73	0.71
2:A:600:FAD:C5B	2:A:600:FAD:C8A	2.60	0.70
1:B:552:GLN:NE2	1:B:552:GLN:H	1.90	0.68
1:A:457:THR:HG21	4:A:2082:HOH:O	1.92	0.68
2:B:600:FAD:C5B	2:B:600:FAD:C8A	2.58	0.68
1:A:552:GLN:NE2	1:A:552:GLN:H	1.92	0.67
1:B:521:ASN:O	1:B:522:SER:HB2	1.94	0.67
1:A:79:ASN:ND2	1:A:82:ASP:H	1.91	0.67
1:A:428:ILE:HD11	1:A:503:TYR:HB3	1.75	0.67
2:B:600:FAD:H9	2:B:600:FAD:O2'	1.94	0.67
1:A:443:THR:HG21	1:A:469:VAL:HG21	1.77	0.66
1:A:217:LEU:CD2	1:B:516:THR:HG23	2.26	0.66
1:B:194:TRP:O	1:B:197:HIS:HD2	1.79	0.65
1:A:188:THR:HB	1:A:189:PRO:CD	2.25	0.65
1:A:149:HIS:ND1	1:A:408:TYR:OH	2.17	0.65
1:A:312:ARG:HG2	1:A:457:THR:HG23	1.78	0.64
1:B:79:ASN:ND2	1:B:82:ASP:H	1.95	0.64
1:B:341:LYS:O	1:B:345:GLN:HG3	1.98	0.64
1:B:471:ILE:HG21	1:B:484:VAL:HG13	1.78	0.64
1:B:443:THR:HG21	1:B:469:VAL:HG21	1.81	0.63
1:B:161:ARG:HG3	4:B:2005:HOH:O	1.97	0.62
1:A:253:LEU:HD11	1:B:253:LEU:HD21	1.81	0.62
1:A:282:THR:HG22	1:A:352:ASN:ND2	2.15	0.61
1:B:149:HIS:ND1	1:B:408:TYR:OH	2.16	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:HIS:CE1	1:B:408:TYR:HE2	2.19	0.61
1:B:310:THR:HG22	1:B:459:THR:HG22	1.82	0.61
1:A:516:THR:HG23	1:B:217:LEU:CD2	2.31	0.61
1:A:531:LEU:HD22	1:B:531:LEU:HD22	1.82	0.61
1:B:187:TYR:O	1:B:307:ASN:HB2	2.01	0.60
1:A:167:ASP:OD1	1:A:186:GLY:HA3	2.02	0.59
1:A:478:LEU:HD12	1:A:478:LEU:H	1.67	0.59
1:B:79:ASN:C	1:B:79:ASN:HD22	2.10	0.59
1:A:188:THR:CB	1:A:189:PRO:CD	2.81	0.59
1:A:468:ILE:HD11	3:A:601:EUG:H92	1.84	0.59
1:B:188:THR:HB	1:B:189:PRO:CD	2.32	0.59
1:B:357:LEU:HD11	1:B:368:TRP:HB2	1.84	0.59
1:B:167:ASP:OD1	1:B:186:GLY:HA3	2.03	0.59
1:B:478:LEU:HD12	1:B:478:LEU:H	1.67	0.59
1:A:152:HIS:HD2	4:A:2096:HOH:O	1.85	0.58
1:A:214:MET:HE1	1:B:517:TYR:OH	2.04	0.58
1:A:149:HIS:CE1	1:A:408:TYR:HE2	2.22	0.58
1:B:516:THR:HG21	4:B:2100:HOH:O	2.02	0.58
1:B:552:GLN:H	1:B:552:GLN:HE21	1.51	0.58
1:B:545:LYS:HE2	2:B:600:FAD:O2B	2.04	0.57
1:A:332:GLU:HB3	1:A:333:PRO:HD2	1.85	0.57
1:B:312:ARG:HG2	1:B:457:THR:HG23	1.86	0.57
1:A:518:ASN:O	1:A:519:TRP:C	2.45	0.57
1:B:149:HIS:HE1	1:B:408:TYR:HE2	1.53	0.57
1:A:57:THR:HG22	1:A:74:ILE:HD11	1.86	0.57
1:A:349:GLY:N	1:A:352:ASN:HD21	1.92	0.57
1:B:188:THR:CB	1:B:189:PRO:CD	2.83	0.57
1:A:195:MET:HE1	1:B:195:MET:SD	2.45	0.57
1:A:552:GLN:H	1:A:552:GLN:HE21	1.50	0.57
1:B:332:GLU:HB3	1:B:333:PRO:HD2	1.87	0.56
1:A:14:PRO:HG3	1:A:558:TRP:CZ2	2.40	0.56
1:A:217:LEU:HD23	1:B:516:THR:HG23	1.86	0.56
1:A:149:HIS:HE1	1:A:408:TYR:HE2	1.53	0.56
1:B:297:ARG:HB3	1:B:298:PRO:CD	2.36	0.56
1:A:102:ILE:HG22	1:A:104:ARG:HG3	1.87	0.55
1:A:194:TRP:O	1:A:197:HIS:HD2	1.89	0.55
1:A:102:ILE:HG12	1:A:175:SER:HB2	1.89	0.55
1:B:385:PHE:HB3	1:B:386:PRO:HD2	1.89	0.54
1:B:428:ILE:HD11	1:B:503:TYR:HB3	1.88	0.54
1:A:471:ILE:HG21	1:A:484:VAL:HG13	1.89	0.54
1:A:341:LYS:O	1:A:345:GLN:HG3	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:THR:CG2	1:A:513:ILE:HD12	2.37	0.54
1:A:513:ILE:O	1:A:516:THR:HB	2.08	0.54
1:B:505:THR:CG2	1:B:513:ILE:HD12	2.37	0.54
1:A:197:HIS:HE1	1:A:251:ASP:OD2	1.90	0.54
1:A:78:ARG:HB2	1:A:82:ASP:OD2	2.08	0.54
2:B:600:FAD:O2'	2:B:600:FAD:C9	2.56	0.53
1:B:197:HIS:HE1	1:B:251:ASP:OD2	1.91	0.53
1:A:385:PHE:HB3	1:A:386:PRO:HD2	1.90	0.53
4:A:2012:HOH:O	1:B:526:ARG:HB3	2.09	0.53
1:B:357:LEU:CD1	1:B:368:TRP:HB2	2.39	0.53
1:A:7:PHE:HB3	4:A:2002:HOH:O	2.08	0.53
1:A:93:PHE:O	1:A:94:SER:HB2	2.07	0.53
1:A:505:THR:HG23	4:A:2123:HOH:O	2.08	0.52
1:B:79:ASN:HD22	1:B:82:ASP:H	1.57	0.52
1:B:102:ILE:HG12	1:B:175:SER:HB2	1.90	0.52
1:B:149:HIS:CE1	1:B:408:TYR:CE2	2.97	0.52
1:B:513:ILE:O	1:B:516:THR:HB	2.09	0.52
1:B:518:ASN:O	1:B:519:TRP:C	2.52	0.52
1:A:480:GLN:O	1:A:484:VAL:HG23	2.08	0.52
1:A:438:MET:HG2	1:A:500:TRP:HH2	1.75	0.52
1:B:57:THR:HG22	1:B:74:ILE:HD11	1.91	0.51
1:A:79:ASN:C	1:A:79:ASN:HD22	2.18	0.51
1:B:417:LEU:HB3	1:B:418:PRO:HD2	1.92	0.51
1:B:14:PRO:HG3	1:B:558:TRP:CZ2	2.46	0.51
1:B:282:THR:HG22	1:B:352:ASN:ND2	2.25	0.51
1:B:468:ILE:HD11	3:B:601:EUG:C9	2.41	0.50
1:A:149:HIS:CE1	1:A:408:TYR:CE2	3.00	0.50
1:A:24:PHE:HD1	1:A:25:ILE:HD12	1.76	0.50
1:A:189:PRO:CG	1:A:270:MET:HE1	2.37	0.50
1:A:346:LEU:O	1:A:347:ASN:HB2	2.12	0.50
1:B:133:VAL:HG11	1:B:160:LEU:HD13	1.94	0.49
1:B:516:THR:HG22	1:B:517:TYR:CD1	2.47	0.49
1:A:521:ASN:O	1:A:522:SER:HB2	2.11	0.49
1:B:346:LEU:O	1:B:347:ASN:HB2	2.11	0.49
1:B:480:GLN:O	1:B:484:VAL:HG23	2.12	0.49
2:B:600:FAD:H8A	2:B:600:FAD:H52A	1.83	0.49
1:A:21:PHE:CZ	1:A:25:ILE:HD13	2.48	0.49
1:A:51:TYR:CE1	1:A:104:ARG:HD3	2.48	0.49
1:A:133:VAL:HG11	1:A:160:LEU:HD13	1.95	0.49
1:A:357:LEU:HD11	1:A:368:TRP:HB2	1.94	0.48
1:A:108:TYR:CZ	1:A:504:ARG:HG2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:LEU:CD1	1:A:368:TRP:HB2	2.44	0.48
1:B:24:PHE:HD1	1:B:25:ILE:HD12	1.78	0.48
1:B:93:PHE:O	1:B:94:SER:HB2	2.14	0.48
1:B:59:ASP:OD2	1:B:62:HIS:HA	2.13	0.48
1:A:195:MET:SD	1:B:195:MET:HE1	2.54	0.47
1:A:477:ASP:O	1:A:481:LYS:HG3	2.14	0.47
1:A:63:VAL:HG12	1:A:473:PHE:CZ	2.49	0.47
1:A:387:GLU:HG2	4:A:2091:HOH:O	2.15	0.47
1:B:297:ARG:HB3	1:B:298:PRO:HD3	1.96	0.47
1:A:79:ASN:HD22	1:A:82:ASP:H	1.62	0.47
1:A:427:PRO:HA	1:A:502:GLU:HA	1.95	0.47
1:B:438:MET:HG2	1:B:500:TRP:HH2	1.80	0.47
1:B:484:VAL:O	1:B:487:LEU:HB3	2.15	0.47
1:A:253:LEU:HD21	1:B:253:LEU:HD11	1.96	0.46
1:A:516:THR:HG23	1:B:217:LEU:HD23	1.97	0.46
1:B:238:ILE:HG22	1:B:238:ILE:O	2.14	0.46
1:A:417:LEU:HB3	1:A:418:PRO:HD2	1.97	0.46
1:B:312:ARG:HD3	1:B:354:TYR:CE1	2.49	0.46
1:A:519:TRP:CH2	1:B:211:ARG:HD3	2.50	0.46
1:B:51:TYR:CE1	1:B:104:ARG:HD3	2.50	0.46
1:B:188:THR:HB	1:B:189:PRO:HD3	1.96	0.46
1:A:253:LEU:CD1	1:B:253:LEU:HD21	2.44	0.46
1:B:468:ILE:HD11	3:B:601:EUG:H93	1.98	0.46
1:A:516:THR:HG22	1:A:517:TYR:CD1	2.50	0.46
1:A:282:THR:HG22	1:A:352:ASN:HD22	1.82	0.45
1:B:131:LEU:HD11	1:B:143:GLU:HG3	1.98	0.45
1:B:24:PHE:CD1	1:B:25:ILE:HD12	2.52	0.45
1:A:244:TYR:OH	1:B:195:MET:HG2	2.16	0.45
1:A:56:HIS:HB2	1:A:74:ILE:HD13	1.99	0.45
1:A:468:ILE:HD11	3:A:601:EUG:C9	2.46	0.45
1:B:21:PHE:CZ	1:B:25:ILE:HD13	2.51	0.45
1:B:31:ILE:HD13	1:B:85:SER:HB3	1.99	0.45
1:A:24:PHE:CD1	1:A:25:ILE:HD12	2.52	0.45
1:A:188:THR:HB	1:A:189:PRO:HD2	1.98	0.45
1:A:361:GLU:HB3	1:A:362:PRO:HD3	1.99	0.45
1:B:78:ARG:HB2	1:B:82:ASP:OD2	2.17	0.45
1:B:90:ALA:HB1	1:B:95:PHE:O	2.18	0.44
1:B:108:TYR:CZ	1:B:504:ARG:HG2	2.52	0.44
1:B:189:PRO:CG	1:B:270:MET:HE1	2.44	0.44
1:A:98:TRP:CD2	1:A:113:PRO:HA	2.52	0.44
1:B:541:ILE:O	1:B:542:ALA:C	2.60	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLY:HA3	1:A:359:GLY:O	2.17	0.44
1:A:187:TYR:O	1:A:307:ASN:HB2	2.16	0.44
1:A:214:MET:SD	1:A:245:GLY:HA2	2.57	0.44
1:B:224:GLU:CD	1:B:224:GLU:H	2.26	0.44
1:B:114:ARG:NH1	1:B:511:ASP:OD2	2.50	0.44
1:B:112:ALA:O	1:B:507:LEU:HD11	2.17	0.44
1:B:378:ILE:O	1:B:381:VAL:HG12	2.18	0.43
1:A:417:LEU:O	1:A:418:PRO:C	2.60	0.43
1:A:210:LEU:C	1:A:210:LEU:HD23	2.44	0.43
1:A:211:ARG:HG2	1:B:519:TRP:CE3	2.54	0.43
1:A:312:ARG:HD3	1:A:354:TYR:CE1	2.53	0.43
1:B:448:GLN:O	1:B:449:GLU:C	2.59	0.43
1:A:195:MET:SD	1:B:195:MET:SD	3.17	0.43
1:B:152:HIS:HD2	4:B:2085:HOH:O	2.01	0.43
1:A:195:MET:HG2	1:B:244:TYR:OH	2.19	0.42
1:B:357:LEU:HB3	1:B:364:ARG:HG2	2.01	0.42
1:B:332:GLU:HB3	1:B:333:PRO:CD	2.49	0.42
1:B:98:TRP:CD2	1:B:113:PRO:HA	2.54	0.42
1:A:80:VAL:O	1:A:81:ALA:C	2.60	0.42
1:A:549:TRP:CH2	1:A:558:TRP:HB3	2.54	0.42
1:A:102:ILE:CG1	1:A:175:SER:HB2	2.48	0.42
1:B:177:LEU:HB2	1:B:265:ILE:HG22	2.01	0.42
1:B:491:LEU:HD23	1:B:491:LEU:HA	1.93	0.42
1:B:79:ASN:ND2	1:B:79:ASN:C	2.78	0.42
1:A:387:GLU:HB2	4:A:2091:HOH:O	2.18	0.42
1:B:90:ALA:O	1:B:94:SER:N	2.53	0.42
1:B:385:PHE:HB3	1:B:386:PRO:CD	2.50	0.42
1:B:13:PRO:HG3	1:B:95:PHE:CE1	2.55	0.41
1:A:28:ILE:O	1:A:32:VAL:HG22	2.20	0.41
1:A:253:LEU:HD21	1:B:253:LEU:CG	2.49	0.41
1:A:142:VAL:HG22	1:A:146:VAL:HG21	2.02	0.41
1:A:257:SER:HA	4:A:2069:HOH:O	2.20	0.41
1:A:398:ARG:NH1	1:A:410:GLU:OE2	2.50	0.41
1:B:177:LEU:HD12	1:B:177:LEU:C	2.45	0.41
1:A:188:THR:HB	1:A:189:PRO:HD3	2.00	0.41
1:A:238:ILE:O	1:A:238:ILE:HG22	2.19	0.41
1:A:310:THR:HG22	1:A:459:THR:HG22	2.03	0.41
1:A:101:SER:O	1:A:124:GLY:HA3	2.20	0.41
1:A:253:LEU:CG	1:B:253:LEU:HD21	2.50	0.41
1:B:95:PHE:CE1	1:B:119:VAL:HG23	2.55	0.41
1:B:361:GLU:N	1:B:362:PRO:HD2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:O	1:A:90:ALA:C	2.63	0.41
1:A:195:MET:CE	1:B:195:MET:SD	3.08	0.41
1:A:541:ILE:O	1:A:542:ALA:C	2.62	0.41
1:A:144:PRO:HD3	1:A:263:THR:O	2.21	0.41
2:A:600:FAD:H2'	2:A:600:FAD:H5'2	1.87	0.40
1:B:71:ALA:HB2	1:B:120:VAL:HG23	2.03	0.40
1:B:427:PRO:HA	1:B:502:GLU:HA	2.03	0.40
1:A:425:PHE:CD2	1:A:427:PRO:HD3	2.56	0.40
1:A:224:GLU:H	1:A:224:GLU:CD	2.29	0.40
1:B:51:TYR:CE1	1:B:171:LEU:HD13	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:VAL:O	1:B:391:GLU:OE2[6_655]	2.01	0.19

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	546/560 (98%)	527 (96%)	18 (3%)	1 (0%)	43	58
1	B	546/560 (98%)	524 (96%)	21 (4%)	1 (0%)	43	58
All	All	1092/1120 (98%)	1051 (96%)	39 (4%)	2 (0%)	43	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	418	PRO
1	A	418	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	469/480 (98%)	435 (93%)	34 (7%)	13	23
1	B	469/480 (98%)	435 (93%)	34 (7%)	13	23
All	All	938/960 (98%)	870 (93%)	68 (7%)	13	23

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	8	ARG
1	A	25	ILE
1	A	30	ARG
1	A	41	SER
1	A	78	ARG
1	A	79	ASN
1	A	114	ARG
1	A	128	ASN
1	A	142	VAL
1	A	177	LEU
1	A	200	MET
1	A	217	LEU
1	A	297	ARG
1	A	301	LEU
1	A	303	MET
1	A	314	ILE
1	A	330	ARG
1	A	331	THR
1	A	336	ASP
1	A	344	LYS
1	A	391	GLU
1	A	412	LYS
1	A	418	PRO
1	A	448	GLN
1	A	457	THR
1	A	472	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	478	LEU
1	A	503	TYR
1	A	504	ARG
1	A	505	THR
1	A	516	THR
1	A	552	GLN
1	A	554	SER
1	B	7	PHE
1	B	8	ARG
1	B	25	ILE
1	B	41	SER
1	B	78	ARG
1	B	79	ASN
1	B	114	ARG
1	B	128	ASN
1	B	142	VAL
1	B	149	HIS
1	B	177	LEU
1	B	200	MET
1	B	297	ARG
1	B	301	LEU
1	B	303	MET
1	B	314	ILE
1	B	330	ARG
1	B	331	THR
1	B	336	ASP
1	B	344	LYS
1	B	381	VAL
1	B	391	GLU
1	B	412	LYS
1	B	418	PRO
1	B	432	SER
1	B	448	GLN
1	B	457	THR
1	B	472	VAL
1	B	478	LEU
1	B	503	TYR
1	B	505	THR
1	B	516	THR
1	B	552	GLN
1	B	554	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	84	GLN
1	A	128	ASN
1	A	152	HIS
1	A	197	HIS
1	A	240	HIS
1	A	277	GLN
1	A	352	ASN
1	A	485	GLN
1	A	520	ASN
1	A	552	GLN
1	B	79	ASN
1	B	128	ASN
1	B	152	HIS
1	B	197	HIS
1	B	240	HIS
1	B	352	ASN
1	B	419	ASN
1	B	520	ASN
1	B	552	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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
2	FAD	A	600	-	58,58,58	2.33	10 (17%)	85,89,89	1.64	25 (29%)
3	EUG	B	601	-	11,11,12	0.71	0	14,14,15	2.27	2 (14%)
3	EUG	A	601	-	11,11,12	0.82	0	14,14,15	2.48	3 (21%)
2	FAD	B	600	-	58,58,58	2.24	10 (17%)	85,89,89	1.57	18 (21%)

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
2	FAD	A	600	-	-	10/34/50/50	0/6/6/6
3	EUG	B	601	-	-	2/4/4/5	0/1/1/1
3	EUG	A	601	-	-	2/4/4/5	0/1/1/1
2	FAD	B	600	-	-	12/34/50/50	0/6/6/6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	P-O3P	-13.48	1.44	1.59
2	B	600	FAD	P-O3P	-12.73	1.45	1.59
2	A	600	FAD	PA-O2A	-4.52	1.34	1.55
2	B	600	FAD	O5'-C5'	4.19	1.60	1.44
2	A	600	FAD	P-O2P	-4.03	1.36	1.55
2	B	600	FAD	PA-O2A	-3.89	1.37	1.55
2	A	600	FAD	O5'-C5'	3.40	1.57	1.44
2	A	600	FAD	O2-C2	-3.25	1.18	1.24
2	B	600	FAD	C1'-C2'	3.12	1.57	1.52
2	B	600	FAD	P-O2P	-3.05	1.41	1.55
2	B	600	FAD	O2-C2	-2.64	1.19	1.24
2	B	600	FAD	O4B-C1B	2.56	1.47	1.42
2	B	600	FAD	PA-O3P	-2.40	1.56	1.59
2	A	600	FAD	C6-C7	-2.34	1.36	1.39
2	A	600	FAD	C2-N1	-2.34	1.31	1.36
2	B	600	FAD	C2-N3	2.33	1.44	1.39
2	A	600	FAD	C2-N3	2.06	1.43	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	FAD	C5'-C4'	2.06	1.54	1.51
2	A	600	FAD	C4A-N9A	2.01	1.41	1.37
2	A	600	FAD	C1'-C2'	2.01	1.55	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	EUG	C9-O3-C3	7.67	128.76	117.51
3	A	601	EUG	C9-O3-C3	6.85	127.56	117.51
3	A	601	EUG	O3-C3-C4	5.01	122.07	114.55
2	B	600	FAD	O3P-P-O1P	3.87	122.35	110.70
2	A	600	FAD	C2A-N1A-C6A	3.56	124.58	118.73
2	B	600	FAD	C5X-C9A-N10	-3.46	114.84	117.97
2	B	600	FAD	O5B-PA-O1A	-3.42	95.36	108.94
2	A	600	FAD	O3P-P-O1P	3.29	120.60	110.70
2	A	600	FAD	C4X-C10-N10	3.14	120.98	116.48
2	A	600	FAD	C4-C4X-N5	3.06	122.44	118.21
2	B	600	FAD	C4X-C10-N10	2.99	120.77	116.48
2	A	600	FAD	O5B-PA-O1A	-2.98	97.13	108.94
3	A	601	EUG	O3-C3-C2	-2.97	118.96	124.08
2	B	600	FAD	C4-N3-C2	-2.89	120.50	125.64
2	A	600	FAD	O2P-P-O5'	2.84	120.43	107.57
2	A	600	FAD	O2A-PA-O1A	2.76	125.31	112.44
2	A	600	FAD	C10-C4X-N5	-2.74	119.21	124.81
2	B	600	FAD	C10-C4X-N5	-2.74	119.21	124.81
2	A	600	FAD	C2B-C1B-N9A	2.66	119.92	113.30
2	B	600	FAD	C4-C4X-N5	2.60	121.81	118.21
3	B	601	EUG	O3-C3-C4	2.58	118.42	114.55
2	A	600	FAD	O4-C4-N3	-2.56	115.30	120.11
2	A	600	FAD	N3A-C2A-N1A	-2.50	124.80	128.58
2	B	600	FAD	O4B-C4B-C5B	-2.47	101.43	109.33
2	B	600	FAD	C2B-C1B-N9A	2.43	119.35	113.30
2	A	600	FAD	C4A-N9A-C1B	-2.41	120.99	126.63
2	B	600	FAD	C9A-C5X-N5	2.40	125.00	122.45
2	A	600	FAD	C5X-C9A-N10	-2.40	115.80	117.97
2	B	600	FAD	C4A-N9A-C1B	-2.39	121.04	126.63
2	A	600	FAD	C1B-N9A-C8A	2.37	132.35	127.09
2	A	600	FAD	O5'-P-O1P	-2.36	99.59	108.94
2	B	600	FAD	O2P-P-O5'	2.32	118.09	107.57
2	A	600	FAD	C4-N3-C2	-2.30	121.55	125.64
2	B	600	FAD	C5'-C4'-C3'	-2.30	107.88	112.22
2	A	600	FAD	C10-N1-C2	2.29	121.81	116.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	O2A-PA-O3P	-2.22	101.26	107.27
2	A	600	FAD	C5'-C4'-C3'	-2.22	108.03	112.22
2	B	600	FAD	O5B-C5B-C4B	-2.21	101.46	108.99
2	B	600	FAD	O4'-C4'-C3'	2.20	114.40	109.25
2	A	600	FAD	C9-C8-C7	-2.18	116.48	119.69
2	A	600	FAD	C4'-C3'-C2'	-2.17	109.95	113.57
2	B	600	FAD	O4-C4-N3	-2.13	116.11	120.11
2	B	600	FAD	C9-C9A-N10	2.10	124.68	121.85
2	A	600	FAD	C9A-C9-C8	2.10	123.45	119.22
2	B	600	FAD	N6A-C6A-N1A	2.09	123.03	118.38
2	A	600	FAD	O2P-P-O3P	-2.08	101.65	107.27
2	A	600	FAD	O4B-C4B-C5B	-2.04	102.81	109.33
2	A	600	FAD	N6A-C6A-N1A	2.02	122.88	118.38

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C5B-O5B-PA-O1A
2	A	600	FAD	C5B-O5B-PA-O2A
2	A	600	FAD	C5B-O5B-PA-O3P
2	A	600	FAD	C5'-O5'-P-O2P
2	A	600	FAD	C5'-O5'-P-O3P
2	B	600	FAD	C5B-O5B-PA-O1A
2	B	600	FAD	C5B-O5B-PA-O2A
2	B	600	FAD	C5B-O5B-PA-O3P
2	B	600	FAD	P-O3P-PA-O5B
2	B	600	FAD	C5'-O5'-P-O1P
2	B	600	FAD	C5'-O5'-P-O2P
2	B	600	FAD	C5'-O5'-P-O3P
3	A	601	EUG	C2-C3-O3-C9
3	B	601	EUG	C2-C3-O3-C9
3	A	601	EUG	C4-C3-O3-C9
3	B	601	EUG	C4-C3-O3-C9
2	B	600	FAD	C3'-C4'-C5'-O5'
2	A	600	FAD	C4'-C5'-O5'-P
2	B	600	FAD	O4B-C4B-C5B-O5B
2	B	600	FAD	C3B-C4B-C5B-O5B
2	B	600	FAD	C4'-C5'-O5'-P
2	A	600	FAD	P-O3P-PA-O5B
2	A	600	FAD	P-O3P-PA-O1A
2	A	600	FAD	O4B-C4B-C5B-O5B

Continued on next page...

Continued from previous page...

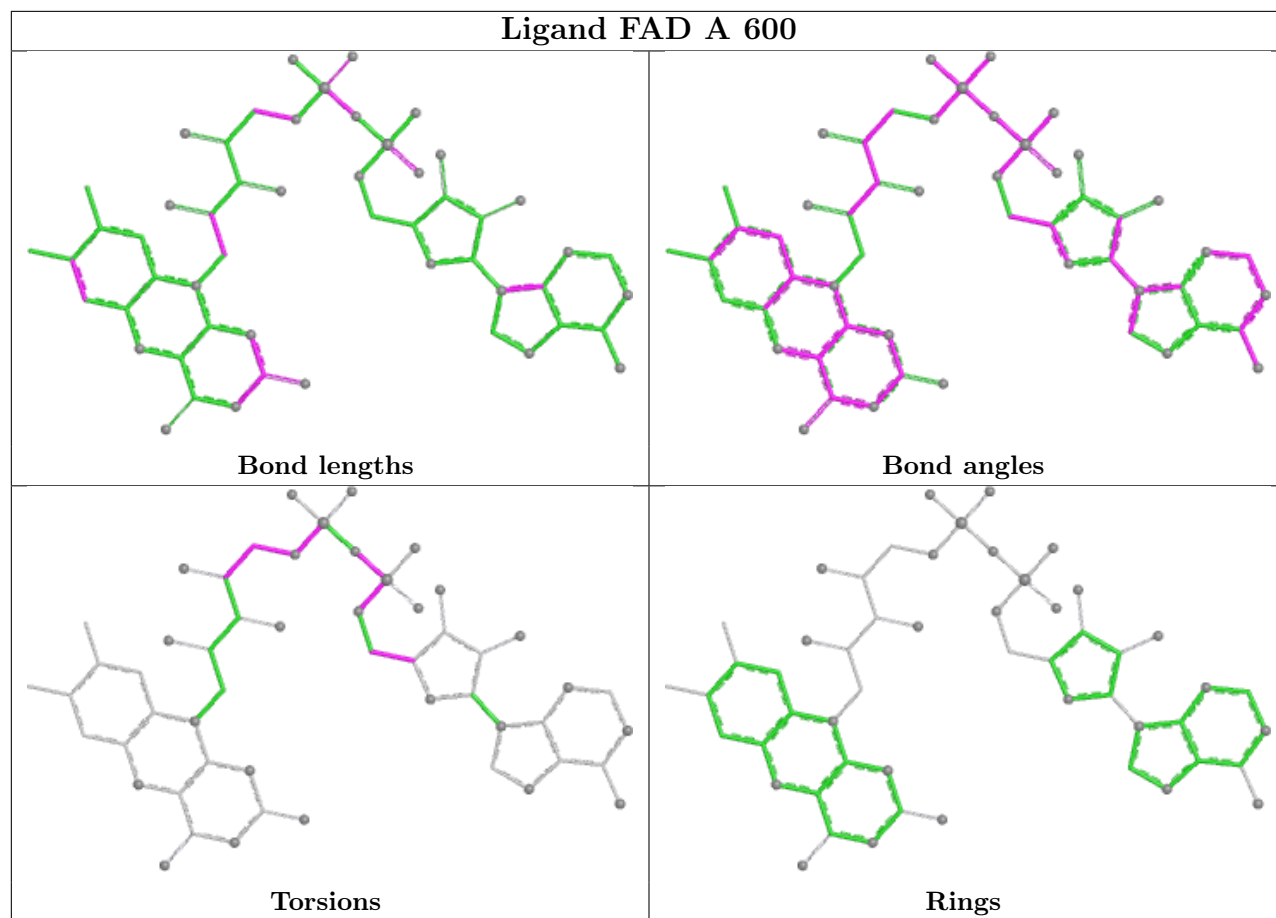
Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C3'-C4'-C5'-O5'
2	B	600	FAD	PA-O3P-P-O2P

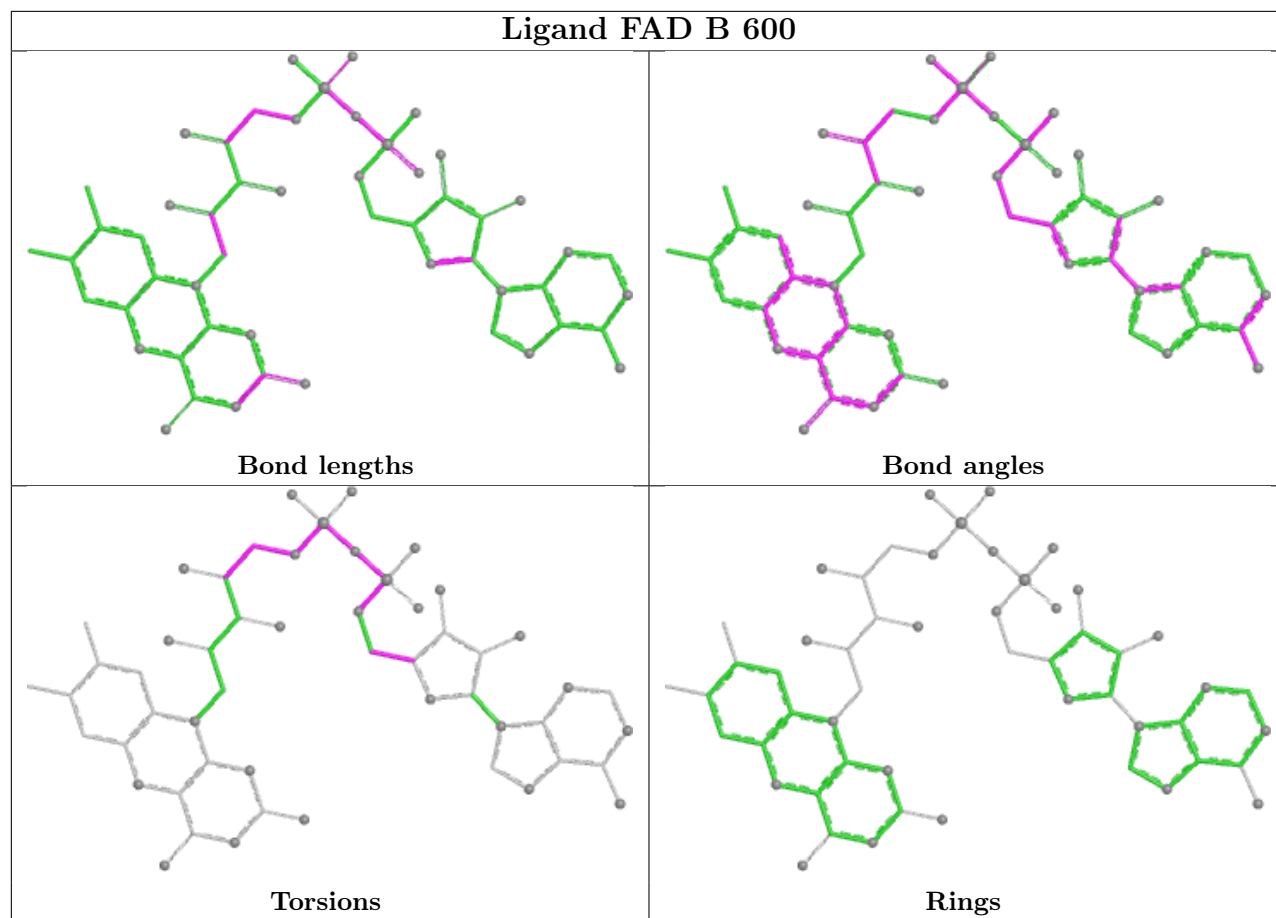
There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	5	0
3	B	601	EUG	2	0
3	A	601	EUG	2	0
2	B	600	FAD	8	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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.