



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 10:32 PM BST

PDB ID : 1DZN
Title : Asp170Ser mutant of vanillyl-alcohol oxidase
Authors : Van Den heuvel, R.H.H.; Fraaije, M.W.; Van Berkel, W.J.H.; Mattevi, A.
Deposited on : 2000-03-05
Resolution : 2.80 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 : 2.13.1
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) : 2.13.1

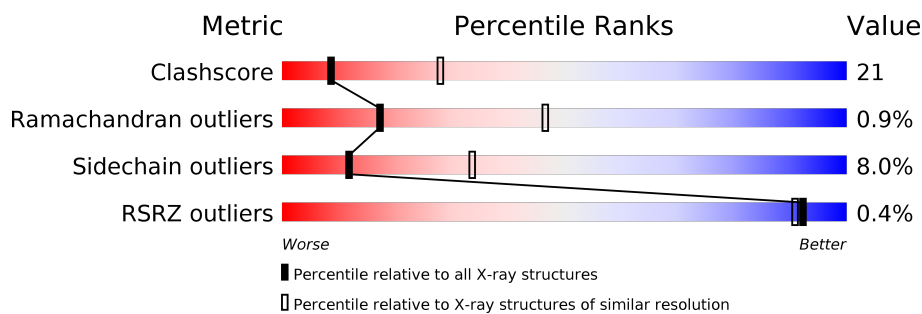
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	560	 57% 34% 6% . .
1	B	560	 54% 35% 7% . .

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 8821 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.

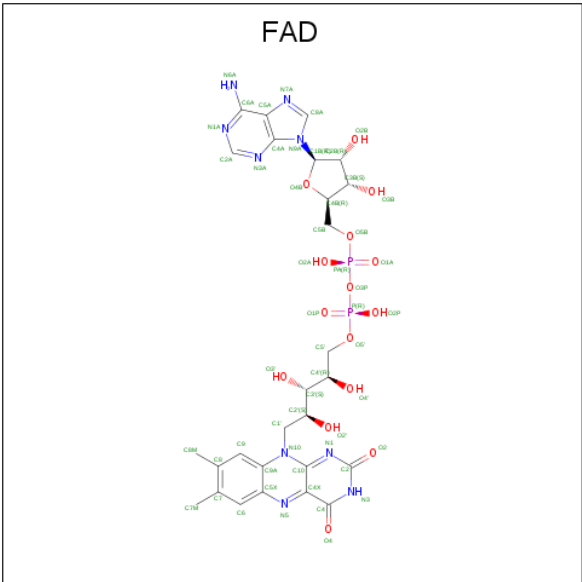
- Molecule 1 is a protein called VANILLYL-ALCOHOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	0	0
			4315	2774	731	787	23			
1	B	550	Total	C	N	O	S	0	0	0
			4316	2775	731	787	23			

There are 5 discrepancies between the modelled and reference sequences:

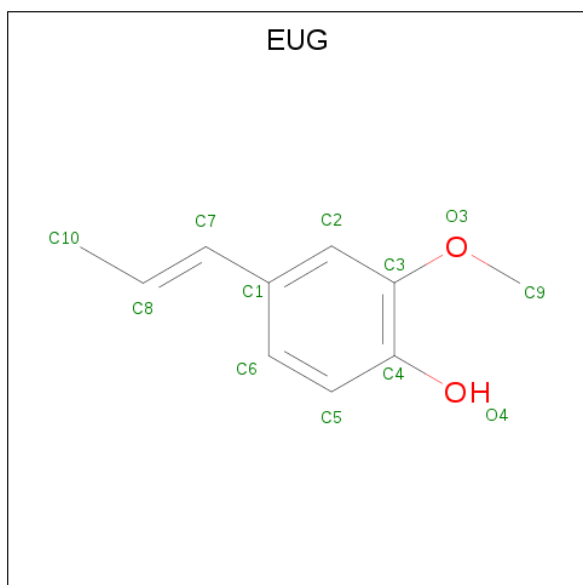
Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ALA	GLU	conflict	UNP P56216
B	6	ALA	GLU	conflict	UNP P56216
A	274	GLY	ARG	conflict	UNP P56216
B	274	GLY	ARG	conflict	UNP P56216
B	170	SER	ASP	engineered mutation	UNP P56216

- 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 2-methoxy-4-[(1E)-prop-1-en-1-yl]phenol (three-letter code: EUG) (formula: $C_{10}H_{12}O_2$).



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		

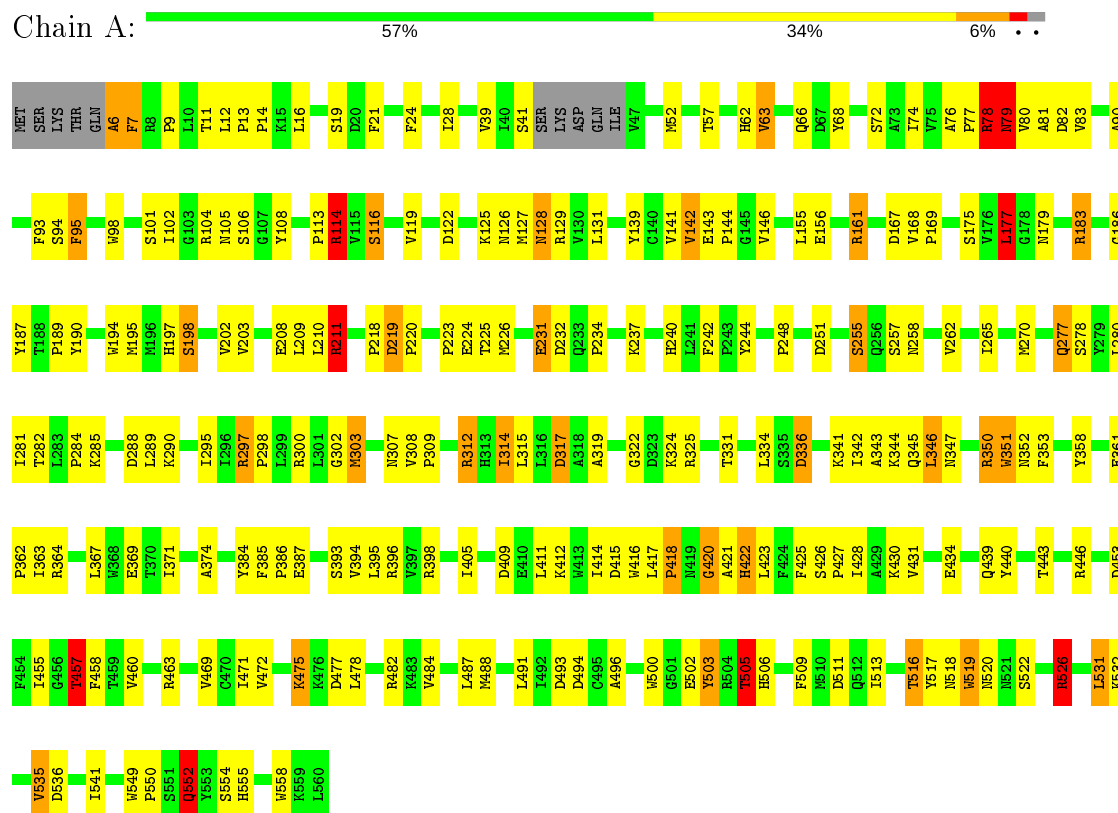
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		
4	B	32	Total	O	0	0
			32	32		

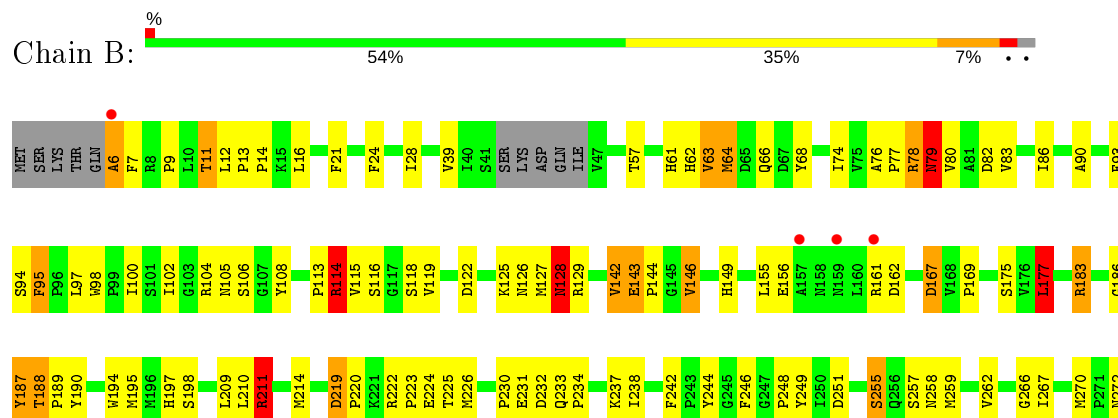
3 Residue-property plots

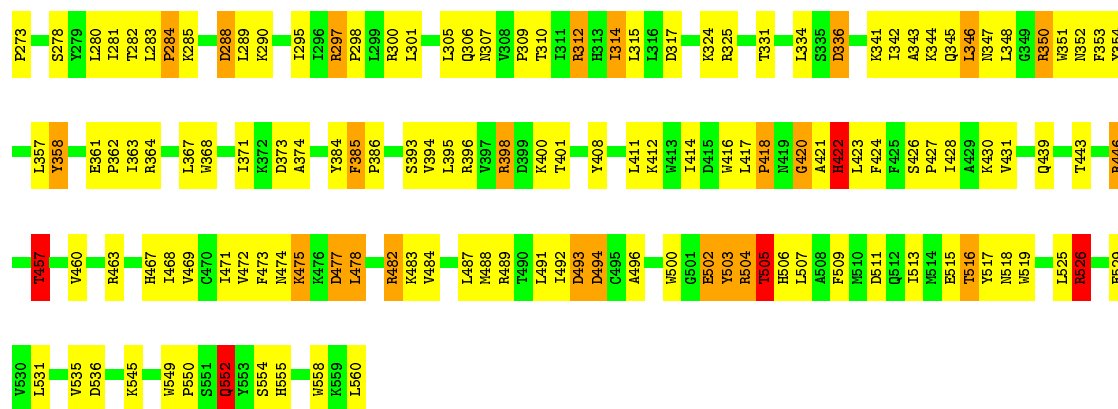
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: VANILLYL-ALCOHOL OXIDASE



• Molecule 1: VANILLYL-ALCOHOL OXIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	131.33Å 131.33Å 134.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 31.65 – 2.80	Depositor EDS
% Data completeness (in resolution range)	83.7 (20.00-2.80) 82.9 (31.65-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.227 , 0.291 0.222 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h 0.038 for -l,-k,-h 0.031 for -h,-l,-k 0.024 for -h,l,k 0.056 for -h,k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8821	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: EUG, 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	0.66	0/4434	1.87	94/6032 (1.6%)
1	B	0.67	0/4435	1.85	83/6034 (1.4%)
All	All	0.67	0/8869	1.86	177/12066 (1.5%)

There are no bond length outliers.

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	ARG	CD-NE-CZ	38.37	177.31	123.60
1	B	398	ARG	CD-NE-CZ	31.00	167.00	123.60
1	B	211	ARG	CD-NE-CZ	19.93	151.50	123.60
1	A	211	ARG	CD-NE-CZ	19.68	151.16	123.60
1	B	446	ARG	NE-CZ-NH1	19.28	129.94	120.30
1	A	526	ARG	CD-NE-CZ	18.93	150.10	123.60
1	A	526	ARG	NE-CZ-NH2	17.51	129.05	120.30
1	B	526	ARG	CD-NE-CZ	15.06	144.69	123.60
1	B	526	ARG	NE-CZ-NH1	-15.00	112.80	120.30
1	B	526	ARG	NE-CZ-NH2	14.17	127.39	120.30
1	A	211	ARG	NE-CZ-NH2	13.89	127.25	120.30
1	B	446	ARG	NE-CZ-NH2	-13.41	113.59	120.30
1	B	325	ARG	NE-CZ-NH2	13.11	126.86	120.30
1	B	211	ARG	NE-CZ-NH1	-13.03	113.78	120.30
1	A	232	ASP	CB-CG-OD1	12.11	129.20	118.30
1	A	446	ARG	NE-CZ-NH1	11.45	126.03	120.30
1	B	297	ARG	CD-NE-CZ	11.35	139.49	123.60
1	A	325	ARG	NE-CZ-NH2	11.02	125.81	120.30
1	B	312	ARG	NE-CZ-NH2	-10.75	114.92	120.30
1	A	536	ASP	CB-CG-OD1	10.75	127.97	118.30
1	A	211	ARG	NE-CZ-NH1	-10.47	115.06	120.30
1	B	177	LEU	CA-CB-CG	10.44	139.30	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	536	ASP	CB-CG-OD1	10.38	127.64	118.30
1	A	78	ARG	NE-CZ-NH2	-10.03	115.29	120.30
1	A	526	ARG	NE-CZ-NH1	-9.89	115.36	120.30
1	A	6	ALA	C-N-CA	9.57	145.62	121.70
1	B	398	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	B	6	ALA	C-N-CA	9.41	145.22	121.70
1	A	68	TYR	CB-CG-CD1	-9.17	115.50	121.00
1	B	493	ASP	CB-CG-OD1	9.03	126.42	118.30
1	B	104	ARG	CD-NE-CZ	9.02	136.22	123.60
1	A	446	ARG	CD-NE-CZ	8.89	136.04	123.60
1	A	297	ARG	CD-NE-CZ	8.75	135.85	123.60
1	A	177	LEU	CA-CB-CG	8.69	135.29	115.30
1	A	494	ASP	CB-CG-OD1	8.60	126.04	118.30
1	B	114	ARG	CD-NE-CZ	8.55	135.56	123.60
1	A	463	ARG	NE-CZ-NH2	-8.49	116.06	120.30
1	B	78	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	A	183	ARG	CD-NE-CZ	8.42	135.39	123.60
1	A	78	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	A	317	ASP	CB-CG-OD2	8.18	125.66	118.30
1	B	504	ARG	NE-CZ-NH1	-8.13	116.24	120.30
1	B	494	ASP	CB-CG-OD1	7.96	125.47	118.30
1	B	336	ASP	CB-CG-OD1	-7.96	111.14	118.30
1	A	114	ARG	CD-NE-CZ	7.93	134.70	123.60
1	A	104	ARG	CD-NE-CZ	7.86	134.61	123.60
1	A	211	ARG	N-CA-CB	7.85	124.74	110.60
1	A	122	ASP	CB-CG-OD1	7.79	125.31	118.30
1	B	457	THR	N-CA-CB	7.68	124.89	110.30
1	B	143	GLU	OE1-CD-OE2	-7.47	114.34	123.30
1	A	434	GLU	OE1-CD-OE2	7.45	132.24	123.30
1	B	446	ARG	CD-NE-CZ	7.40	133.97	123.60
1	A	300	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	B	6	ALA	CA-C-O	7.37	135.57	120.10
1	A	114	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	B	114	ARG	N-CA-CB	7.32	123.78	110.60
1	B	457	THR	CB-CA-C	-7.28	91.96	111.60
1	A	219	ASP	CB-CG-OD1	7.25	124.83	118.30
1	A	336	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	B	68	TYR	CB-CG-CD1	-7.13	116.72	121.00
1	A	312	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	B	552	GLN	CA-CB-CG	7.08	128.97	113.40
1	A	187	TYR	CB-CG-CD2	-7.05	116.77	121.00
1	B	183	ARG	CD-NE-CZ	7.04	133.46	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	A	255	SER	N-CA-CB	6.96	120.94	110.50
1	A	68	TYR	CB-CG-CD2	6.85	125.11	121.00
1	B	336	ASP	OD1-CG-OD2	6.75	136.12	123.30
1	B	167	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	B	325	ARG	NE-CZ-NH1	-6.71	116.94	120.30
1	A	477	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	211	ARG	CA-CB-CG	6.61	127.94	113.40
1	B	489	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	A	231	GLU	OE1-CD-OE2	6.58	131.19	123.30
1	B	300	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	B	211	ARG	CA-CB-CG	6.51	127.72	113.40
1	A	364	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	B	78	ARG	CD-NE-CZ	6.42	132.58	123.60
1	A	440	TYR	CB-CG-CD2	-6.41	117.15	121.00
1	B	336	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	300	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	6	ALA	O-C-N	-6.31	112.60	122.70
1	A	457	THR	N-CA-CB	6.30	122.26	110.30
1	A	78	ARG	CD-NE-CZ	6.28	132.39	123.60
1	A	122	ASP	OD1-CG-OD2	-6.21	111.51	123.30
1	A	384	TYR	CB-CG-CD2	6.19	124.72	121.00
1	A	336	ASP	OD1-CG-OD2	6.17	135.02	123.30
1	B	312	ARG	NH1-CZ-NH2	6.11	126.12	119.40
1	A	129	ARG	N-CA-C	6.11	127.49	111.00
1	B	364	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	219	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	A	520	ASN	CB-CG-OD1	-6.07	109.46	121.60
1	A	139	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	A	208	GLU	OE1-CD-OE2	-6.02	116.08	123.30
1	B	482	ARG	CD-NE-CZ	6.00	132.00	123.60
1	A	387	GLU	OE1-CD-OE2	-5.99	116.11	123.30
1	A	552	GLN	CA-CB-CG	5.99	126.57	113.40
1	B	258	ASN	O-C-N	-5.97	113.15	122.70
1	B	560	LEU	CA-C-O	-5.94	107.63	120.10
1	B	127	MET	CA-C-O	5.93	132.56	120.10
1	B	484	VAL	CA-CB-CG2	-5.93	102.00	110.90
1	A	422	HIS	N-CA-CB	5.89	121.21	110.60
1	B	79	ASN	N-CA-CB	-5.88	100.02	110.60
1	A	218	PRO	O-C-N	5.86	132.08	122.70
1	A	6	ALA	CA-C-O	5.84	132.37	120.10
1	B	384	TYR	CB-CG-CD2	5.83	124.50	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	312	ARG	CD-NE-CZ	-5.83	115.44	123.60
1	A	336	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	A	484	VAL	CA-CB-CG2	-5.79	102.22	110.90
1	B	358	TYR	CB-CG-CD2	-5.76	117.54	121.00
1	A	19	SER	N-CA-CB	-5.76	101.86	110.50
1	B	373	ASP	CB-CG-OD1	-5.75	113.12	118.30
1	A	232	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	A	183	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	6	ALA	O-C-N	-5.66	113.64	122.70
1	A	114	ARG	N-CA-CB	5.66	120.79	110.60
1	A	409	ASP	CB-CG-OD1	5.64	123.37	118.30
1	A	369	GLU	OE1-CD-OE2	5.63	130.06	123.30
1	B	336	ASP	CA-CB-CG	-5.63	101.02	113.40
1	B	211	ARG	N-CA-CB	5.62	120.72	110.60
1	B	219	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	B	68	TYR	CB-CG-CD2	5.58	124.35	121.00
1	B	249	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	A	434	GLU	CB-CG-CD	-5.57	99.17	114.20
1	A	128	ASN	N-CA-CB	-5.51	100.67	110.60
1	B	122	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	505	THR	CB-CA-C	-5.49	96.78	111.60
1	A	312	ARG	NH1-CZ-NH2	5.49	125.44	119.40
1	B	463	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	536	ASP	CA-C-O	5.47	131.58	120.10
1	A	128	ASN	CB-CA-C	-5.46	99.47	110.40
1	B	129	ARG	N-CA-C	5.46	125.74	111.00
1	B	504	ARG	NH1-CZ-NH2	5.46	125.41	119.40
1	A	535	VAL	CG1-CB-CG2	-5.45	102.18	110.90
1	A	104	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	128	ASN	CB-CA-C	-5.42	99.57	110.40
1	B	297	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	122	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	505	THR	CB-CA-C	-5.38	97.06	111.60
1	B	232	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	139	TYR	CB-CG-CD2	5.36	124.22	121.00
1	A	63	VAL	N-CA-CB	5.35	123.26	111.50
1	A	351	TRP	CA-C-O	-5.33	108.92	120.10
1	B	422	HIS	N-CA-CB	5.32	120.17	110.60
1	A	457	THR	CB-CA-C	-5.30	97.28	111.60
1	A	161	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	128	ASN	N-CA-C	5.28	125.25	111.00
1	A	127	MET	C-N-CA	5.26	134.86	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	B	63	VAL	N-CA-CB	5.25	123.04	111.50
1	A	277	GLN	CA-CB-CG	5.23	124.91	113.40
1	B	493	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	300	ARG	CD-NE-CZ	5.22	130.91	123.60
1	B	246	PHE	O-C-N	-5.22	114.33	123.20
1	B	162	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	232	ASP	CA-C-N	5.21	128.67	117.20
1	A	303	MET	CA-C-O	5.21	131.05	120.10
1	B	127	MET	C-N-CA	5.20	134.70	121.70
1	A	187	TYR	CA-CB-CG	-5.18	103.56	113.40
1	A	232	ASP	CA-C-N	5.18	128.59	117.20
1	A	127	MET	CA-C-O	5.16	130.94	120.10
1	B	288	ASP	CB-CG-OD1	5.16	122.95	118.30
1	B	146	VAL	CA-CB-CG2	-5.14	103.18	110.90
1	B	214	MET	CB-CA-C	5.14	120.68	110.40
1	A	79	ASN	N-CA-CB	-5.12	101.38	110.60
1	B	187	TYR	CA-CB-CG	-5.11	103.69	113.40
1	A	52	MET	CB-CA-C	5.10	120.61	110.40
1	B	515	GLU	OE1-CD-OE2	5.09	129.41	123.30
1	B	477	ASP	CB-CG-OD1	5.06	122.86	118.30
1	B	385	PHE	CB-CG-CD1	5.05	124.33	120.80
1	A	72	SER	N-CA-CB	5.04	118.06	110.50
1	A	168	VAL	CB-CA-C	-5.04	101.82	111.40
1	A	114	ARG	CB-CG-CD	5.04	124.71	111.60
1	A	531	LEU	CA-CB-CG	5.03	126.86	115.30
1	A	552	GLN	CB-CG-CD	5.02	124.65	111.60
1	A	128	ASN	N-CA-C	5.01	124.52	111.00
1	B	64	MET	CA-CB-CG	5.01	121.81	113.30

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	4315	0	4223	175	0
1	B	4316	0	4227	181	0
2	A	53	0	30	9	0
2	B	53	0	30	8	0
3	A	11	0	7	0	0
3	B	11	0	7	2	0
4	A	30	0	0	3	0
4	B	32	0	0	2	0
All	All	8821	0	8524	356	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 21.

All (356) 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	1.74	1.16
2:A:600:FAD:H8A	2:A:600:FAD:H51A	1.17	1.15
2:A:600:FAD:H8A	2:A:600:FAD:C5B	1.85	1.06
2:B:600:FAD:H51A	2:B:600:FAD:H8A	1.08	1.05
2:B:600:FAD:H51A	2:B:600:FAD:C8A	1.99	0.93
1:B:312:ARG:HG2	1:B:457:THR:HG23	1.54	0.86
2:A:600:FAD:C8A	2:A:600:FAD:H51A	2.05	0.85
1:A:385:PHE:HB3	1:A:386:PRO:HD2	1.60	0.82
1:B:14:PRO:HG3	1:B:558:TRP:CZ2	2.17	0.80
1:A:14:PRO:HG3	1:A:558:TRP:CZ2	2.19	0.78
1:B:14:PRO:HG3	1:B:558:TRP:HZ2	1.47	0.77
1:B:79:ASN:ND2	1:B:82:ASP:H	1.84	0.76
2:B:600:FAD:N1	2:B:600:FAD:O3'	2.19	0.76
1:B:385:PHE:HB3	1:B:386:PRO:HD2	1.68	0.76
1:A:6:ALA:HB3	1:A:39:VAL:HG21	1.68	0.75
1:A:79:ASN:ND2	1:A:82:ASP:H	1.85	0.74
1:A:312:ARG:HG2	1:A:457:THR:HG23	1.67	0.74
1:A:14:PRO:HG3	1:A:558:TRP:HZ2	1.52	0.74
1:A:57:THR:HG22	1:A:74:ILE:HD11	1.71	0.73
1:B:478:LEU:H	1:B:478:LEU:HD12	1.54	0.73
1:B:177:LEU:HD21	1:B:262:VAL:HG12	1.71	0.73
1:B:143:GLU:HB3	1:B:144:PRO:HD2	1.69	0.73
1:B:443:THR:HG21	1:B:469:VAL:HG21	1.70	0.72
1:A:367:LEU:HD21	1:B:363:ILE:HD11	1.73	0.70
1:B:6:ALA:HB3	1:B:39:VAL:HG21	1.72	0.70
1:B:385:PHE:HB3	1:B:386:PRO:CD	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:LEU:HB3	1:A:418:PRO:HD2	1.71	0.70
1:B:417:LEU:HB3	1:B:418:PRO:HD2	1.72	0.70
1:B:416:TRP:HB3	1:B:472:VAL:HG21	1.74	0.70
1:A:478:LEU:H	1:A:478:LEU:HD12	1.58	0.69
1:A:297:ARG:HB3	1:A:298:PRO:CD	2.23	0.68
1:A:428:ILE:HD11	1:A:503:TYR:HB3	1.76	0.68
1:B:11:THR:HG21	1:B:116:SER:HB3	1.75	0.68
1:A:443:THR:HG21	1:A:469:VAL:HG21	1.76	0.68
1:A:79:ASN:HD22	1:A:79:ASN:C	1.97	0.68
1:B:282:THR:HG22	1:B:352:ASN:HD22	1.59	0.68
1:A:385:PHE:HB3	1:A:386:PRO:CD	2.24	0.68
1:A:416:TRP:HB3	1:A:472:VAL:HG21	1.74	0.67
1:B:428:ILE:HD11	1:B:503:TYR:HB3	1.77	0.67
2:B:600:FAD:C8A	2:B:600:FAD:C5B	2.64	0.67
1:A:341:LYS:O	1:A:345:GLN:HG3	1.95	0.67
1:A:297:ARG:HG3	1:A:431:VAL:O	1.95	0.67
1:A:282:THR:HG22	1:A:352:ASN:HD22	1.59	0.66
1:B:341:LYS:O	1:B:345:GLN:HG3	1.95	0.66
1:A:177:LEU:HD21	1:A:262:VAL:HG12	1.79	0.65
1:A:190:TYR:CE1	1:A:270:MET:HG3	2.32	0.65
1:B:66:GLN:O	1:B:66:GLN:HG2	1.96	0.65
2:A:600:FAD:O3'	2:A:600:FAD:N1	2.29	0.65
1:A:12:LEU:HB3	1:A:13:PRO:HD2	1.79	0.64
1:B:167:ASP:OD1	1:B:186:GLY:HA3	1.97	0.64
1:A:93:PHE:O	1:A:94:SER:HB2	1.98	0.64
1:A:209:LEU:HD11	1:A:231:GLU:HG3	1.78	0.64
1:A:9:PRO:HG3	1:A:21:PHE:CE2	2.33	0.64
1:A:161:ARG:HH21	1:A:405:ILE:HD11	1.63	0.64
1:B:12:LEU:HB3	1:B:13:PRO:HD2	1.79	0.64
1:B:297:ARG:HG3	1:B:431:VAL:O	1.97	0.64
1:B:242:PHE:CE2	1:B:244:TYR:HB2	2.34	0.63
1:A:361:GLU:N	1:A:362:PRO:HD2	2.14	0.63
1:A:179:ASN:ND2	2:A:600:FAD:O3'	2.31	0.62
1:B:93:PHE:O	1:B:94:SER:HB2	2.00	0.62
1:B:297:ARG:HB3	1:B:298:PRO:CD	2.29	0.62
1:A:6:ALA:HB3	1:A:39:VAL:CG2	2.29	0.61
1:A:242:PHE:CE2	1:A:244:TYR:HB2	2.35	0.61
1:A:411:LEU:O	1:A:414:ILE:HD12	2.00	0.61
1:A:430:LYS:HD2	1:B:237:LYS:HB3	1.83	0.61
1:A:80:VAL:HB	1:A:231:GLU:HG2	1.82	0.60
1:A:516:THR:HG22	1:A:517:TYR:CD1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ILE:HG13	1:B:343:ALA:HB2	1.83	0.60
1:A:66:GLN:HG2	1:A:66:GLN:O	1.99	0.60
1:A:98:TRP:CD2	1:A:113:PRO:HA	2.37	0.60
1:B:297:ARG:HB3	1:B:298:PRO:HD3	1.83	0.60
1:B:393:SER:OG	1:B:396:ARG:HG3	2.01	0.60
1:A:278:SER:OG	1:A:386:PRO:HG3	2.02	0.59
1:B:443:THR:HA	1:B:491:LEU:CD2	2.33	0.59
1:B:284:PRO:O	1:B:350:ARG:HB2	2.03	0.59
1:A:280:LEU:CB	1:A:395:LEU:HD22	2.33	0.59
1:B:142:VAL:HG22	1:B:146:VAL:HG21	1.84	0.59
1:B:317:ASP:OD1	1:B:394:VAL:HG21	2.03	0.58
1:A:11:THR:HG21	1:A:116:SER:HB3	1.85	0.58
1:A:237:LYS:HB3	1:B:430:LYS:HD2	1.84	0.58
1:A:505:THR:HG23	4:A:2021:HOH:O	2.03	0.58
1:B:513:ILE:O	1:B:516:THR:HB	2.03	0.58
1:B:341:LYS:O	1:B:344:LYS:HG2	2.02	0.58
1:A:280:LEU:HB3	1:A:395:LEU:HD22	1.85	0.58
1:A:478:LEU:HB3	1:A:482:ARG:NH2	2.18	0.58
1:A:142:VAL:HG22	1:A:146:VAL:HG21	1.86	0.57
1:B:80:VAL:HB	1:B:231:GLU:HG2	1.85	0.57
1:A:297:ARG:HB3	1:A:298:PRO:HD3	1.86	0.57
1:A:169:PRO:HB2	4:A:2009:HOH:O	2.04	0.57
1:B:9:PRO:HG2	1:B:12:LEU:CD2	2.35	0.57
1:B:312:ARG:HG2	1:B:457:THR:CG2	2.32	0.57
1:B:285:LYS:HB2	1:B:288:ASP:OD2	2.05	0.57
1:A:341:LYS:O	1:A:344:LYS:HG2	2.05	0.56
1:B:427:PRO:HA	1:B:502:GLU:HA	1.86	0.56
1:A:342:ILE:O	1:A:346:LEU:HG	2.06	0.56
1:A:550:PRO:HB2	1:A:552:GLN:NE2	2.19	0.56
1:A:425:PHE:CE2	1:A:427:PRO:HG3	2.41	0.56
1:B:125:LYS:HG2	1:B:126:ASN:OD1	2.04	0.56
1:B:6:ALA:HB3	1:B:39:VAL:CG2	2.35	0.56
1:A:411:LEU:HD23	1:A:414:ILE:CD1	2.36	0.56
1:A:282:THR:HG22	1:A:352:ASN:ND2	2.20	0.56
1:B:361:GLU:N	1:B:362:PRO:HD2	2.21	0.56
1:B:9:PRO:HG3	1:B:21:PHE:CE2	2.40	0.56
1:A:167:ASP:OD1	1:A:186:GLY:HA3	2.06	0.56
1:B:77:PRO:O	1:B:126:ASN:HB2	2.06	0.55
1:B:209:LEU:HD11	1:B:231:GLU:HG3	1.87	0.55
1:B:225:THR:HG21	1:B:234:PRO:HG3	1.89	0.55
1:A:314:ILE:HD11	1:A:343:ALA:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PRO:HG3	1:A:21:PHE:CZ	2.42	0.55
2:A:600:FAD:C8A	2:A:600:FAD:C5B	2.73	0.54
1:A:189:PRO:HG2	1:A:270:MET:HE1	1.89	0.54
1:A:363:ILE:HD11	1:B:367:LEU:HD21	1.88	0.54
1:A:194:TRP:O	1:A:197:HIS:HD2	1.90	0.54
1:A:443:THR:HA	1:A:491:LEU:CD2	2.38	0.54
1:A:439:GLN:HA	1:A:500:TRP:CH2	2.42	0.54
1:A:79:ASN:HD21	1:A:82:ASP:H	1.53	0.54
1:A:13:PRO:HG2	1:A:16:LEU:HD22	1.89	0.54
1:B:187:TYR:O	1:B:307:ASN:HB2	2.08	0.54
1:B:411:LEU:HD23	1:B:414:ILE:CD1	2.38	0.54
1:A:552:GLN:H	1:A:552:GLN:HE21	1.54	0.54
1:B:98:TRP:CD2	1:B:113:PRO:HA	2.43	0.53
1:B:493:ASP:O	1:B:496:ALA:HB3	2.08	0.53
1:B:12:LEU:HB3	1:B:13:PRO:CD	2.38	0.53
1:A:314:ILE:HG13	1:A:343:ALA:HB2	1.90	0.53
1:B:210:LEU:HD23	1:B:211:ARG:N	2.24	0.53
1:B:315:LEU:HD21	1:B:334:LEU:HD12	1.90	0.53
1:B:57:THR:HG22	1:B:74:ILE:HD11	1.91	0.53
1:B:550:PRO:HB2	1:B:552:GLN:NE2	2.24	0.53
1:A:315:LEU:HD21	1:A:334:LEU:HD12	1.90	0.53
1:B:143:GLU:HB3	1:B:144:PRO:CD	2.39	0.53
1:A:312:ARG:HG2	1:A:457:THR:CG2	2.36	0.52
1:A:289:LEU:HD22	1:A:351:TRP:CZ2	2.43	0.52
1:A:367:LEU:O	1:A:371:ILE:HG13	2.10	0.52
1:B:289:LEU:HD22	1:B:351:TRP:CZ2	2.45	0.52
1:B:414:ILE:O	1:B:420:GLY:HA3	2.09	0.52
1:A:248:PRO:HG3	1:B:257:SER:HB2	1.92	0.52
1:A:9:PRO:HG2	1:A:12:LEU:CD2	2.40	0.52
1:B:478:LEU:HB3	1:B:482:ARG:NH2	2.24	0.52
1:B:24:PHE:O	1:B:28:ILE:HG12	2.09	0.52
1:B:282:THR:HG22	1:B:352:ASN:ND2	2.25	0.52
1:B:483:LYS:O	1:B:487:LEU:N	2.37	0.52
1:B:79:ASN:HD22	1:B:79:ASN:C	2.12	0.52
1:B:95:PHE:CE1	1:B:119:VAL:HG23	2.45	0.51
1:A:519:TRP:CZ3	1:B:211:ARG:HG2	2.45	0.51
1:A:317:ASP:OD1	1:A:394:VAL:HG21	2.11	0.51
1:B:414:ILE:HD11	2:B:600:FAD:HM71	1.91	0.51
1:B:219:ASP:OD1	1:B:220:PRO:HD2	2.10	0.51
1:B:266:GLY:O	1:B:267:ILE:HD13	2.10	0.51
1:B:367:LEU:O	1:B:371:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ARG:CG	1:B:457:THR:HG23	2.33	0.51
1:B:280:LEU:HB3	1:B:395:LEU:HD22	1.93	0.51
1:A:114:ARG:NH1	1:A:511:ASP:OD2	2.44	0.51
1:A:102:ILE:HG12	1:A:175:SER:HB2	1.93	0.51
1:A:219:ASP:OD1	1:A:220:PRO:HD2	2.11	0.50
1:B:82:ASP:O	1:B:86:ILE:HG13	2.12	0.50
1:B:398:ARG:HA	1:B:401:THR:HB	1.94	0.50
1:B:421:ALA:HB2	1:B:475:LYS:HG2	1.94	0.50
1:B:421:ALA:HB3	1:B:473:PHE:CZ	2.47	0.50
1:A:393:SER:OG	1:A:396:ARG:HG3	2.11	0.50
1:A:518:ASN:O	1:A:519:TRP:C	2.48	0.50
1:B:545:LYS:HE2	2:B:600:FAD:O2B	2.11	0.50
1:A:161:ARG:NH2	1:A:405:ILE:HD11	2.26	0.50
1:A:421:ALA:HB2	1:A:475:LYS:HG2	1.94	0.50
1:B:183:ARG:O	1:B:503:TYR:HE2	1.95	0.50
1:B:9:PRO:HG3	1:B:21:PHE:CZ	2.47	0.50
1:B:443:THR:HG21	1:B:469:VAL:CG2	2.40	0.50
1:A:302:GLY:O	1:A:303:MET:HB2	2.12	0.50
1:A:77:PRO:O	1:A:126:ASN:HB2	2.12	0.50
1:A:242:PHE:CZ	1:A:244:TYR:HB2	2.47	0.49
1:B:169:PRO:HB2	4:B:2015:HOH:O	2.12	0.49
1:A:12:LEU:HB3	1:A:13:PRO:CD	2.42	0.49
1:B:13:PRO:HG2	1:B:16:LEU:HD22	1.94	0.49
1:A:439:GLN:HA	1:A:500:TRP:CZ3	2.47	0.49
1:A:90:ALA:O	1:A:94:SER:N	2.45	0.49
1:B:357:LEU:HD13	1:B:368:TRP:HB2	1.93	0.49
1:A:531:LEU:HD22	1:B:531:LEU:HD22	1.94	0.49
1:B:108:TYR:O	1:B:506:HIS:HA	2.13	0.49
1:A:143:GLU:O	1:A:144:PRO:C	2.49	0.49
1:B:64:MET:HB2	4:B:2007:HOH:O	2.12	0.49
1:A:189:PRO:HB2	1:A:270:MET:HE3	1.94	0.49
1:A:248:PRO:HG3	1:B:257:SER:CB	2.43	0.49
1:B:79:ASN:ND2	1:B:82:ASP:N	2.57	0.49
1:A:258:ASN:HB2	1:A:541:ILE:O	2.12	0.49
1:B:278:SER:OG	1:B:386:PRO:HG3	2.13	0.49
1:A:488:MET:HG2	1:A:509:PHE:CE2	2.48	0.48
1:A:549:TRP:HB2	1:A:555:HIS:HE1	1.78	0.48
1:B:230:PRO:O	1:B:231:GLU:C	2.51	0.48
1:B:341:LYS:HG2	1:B:344:LYS:NZ	2.28	0.48
1:B:423:LEU:O	1:B:471:ILE:HB	2.13	0.48
1:B:280:LEU:CB	1:B:395:LEU:HD22	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:LEU:HD22	1:B:416:TRP:CZ2	2.48	0.48
1:A:505:THR:HG21	1:A:513:ILE:CD1	2.43	0.48
1:B:194:TRP:O	1:B:197:HIS:HD2	1.96	0.48
1:A:307:ASN:O	1:A:309:PRO:HD3	2.13	0.48
1:A:493:ASP:O	1:A:496:ALA:HB3	2.13	0.48
1:B:341:LYS:HA	1:B:344:LYS:HD3	1.94	0.48
1:B:411:LEU:O	1:B:414:ILE:HD12	2.14	0.48
1:B:342:ILE:O	1:B:346:LEU:HG	2.14	0.48
1:A:79:ASN:ND2	1:A:79:ASN:C	2.66	0.48
1:B:115:VAL:HG13	1:B:558:TRP:CH2	2.48	0.47
1:A:257:SER:HB2	1:B:248:PRO:HG3	1.96	0.47
1:B:516:THR:HG22	1:B:517:TYR:CD1	2.49	0.47
1:A:62:HIS:H	1:A:62:HIS:CD2	2.30	0.47
1:A:95:PHE:CE1	1:A:119:VAL:HG23	2.49	0.47
1:B:354:TYR:CE2	1:B:394:VAL:HG12	2.49	0.47
1:A:277:GLN:HE21	1:A:278:SER:N	2.13	0.47
1:A:513:ILE:O	1:A:516:THR:HB	2.15	0.47
1:B:314:ILE:HD11	1:B:343:ALA:HA	1.97	0.47
1:A:423:LEU:O	1:A:471:ILE:HB	2.14	0.47
1:B:224:GLU:H	1:B:224:GLU:CD	2.18	0.47
1:A:24:PHE:O	1:A:28:ILE:HG12	2.15	0.47
1:A:143:GLU:HB3	1:A:144:PRO:HD2	1.96	0.47
1:A:79:ASN:HD21	1:A:82:ASP:N	2.12	0.47
1:B:259:MET:HE3	1:B:535:VAL:HG21	1.96	0.47
1:B:143:GLU:O	1:B:144:PRO:C	2.53	0.47
1:B:238:ILE:HG22	1:B:238:ILE:O	2.15	0.47
1:B:90:ALA:HB1	1:B:95:PHE:O	2.15	0.47
1:B:190:TYR:CE1	1:B:270:MET:HG3	2.51	0.46
1:B:549:TRP:CH2	1:B:558:TRP:HB3	2.50	0.46
1:B:525:LEU:O	1:B:529:GLU:HG3	2.14	0.46
1:A:455:ILE:HG13	4:A:2025:HOH:O	2.15	0.46
1:B:361:GLU:O	1:B:362:PRO:C	2.53	0.46
1:A:427:PRO:HA	1:A:502:GLU:HA	1.97	0.46
1:A:195:MET:HG2	1:B:244:TYR:OH	2.16	0.46
1:A:285:LYS:HB2	1:A:288:ASP:OD2	2.16	0.46
1:A:341:LYS:HG2	1:A:344:LYS:NZ	2.31	0.46
1:B:346:LEU:O	1:B:347:ASN:HB2	2.15	0.46
1:B:526:ARG:HA	1:B:526:ARG:HD3	1.55	0.46
1:B:149:HIS:CE1	1:B:408:TYR:HE1	2.34	0.46
1:A:210:LEU:HD23	1:A:211:ARG:N	2.31	0.45
1:B:233:GLN:HB3	1:B:234:PRO:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:LEU:O	1:B:492:ILE:C	2.55	0.45
1:A:224:GLU:H	1:A:224:GLU:CD	2.19	0.45
1:B:314:ILE:HD13	1:B:314:ILE:O	2.16	0.45
1:A:346:LEU:O	1:A:347:ASN:HB2	2.17	0.45
1:A:281:ILE:HD12	1:A:353:PHE:HD2	1.80	0.45
1:B:90:ALA:O	1:B:94:SER:N	2.49	0.45
1:A:108:TYR:O	1:A:506:HIS:HA	2.17	0.45
1:A:552:GLN:H	1:A:552:GLN:NE2	2.14	0.45
1:B:518:ASN:O	1:B:519:TRP:C	2.55	0.45
1:A:177:LEU:HD22	1:A:265:ILE:HB	1.98	0.45
1:B:305:LEU:HD23	1:B:305:LEU:HA	1.79	0.45
1:B:549:TRP:HB2	1:B:555:HIS:HE1	1.82	0.45
1:A:211:ARG:HG2	1:B:519:TRP:CZ3	2.52	0.45
1:B:102:ILE:HA	1:B:102:ILE:HD13	1.87	0.45
1:B:443:THR:HA	1:B:491:LEU:HD21	1.98	0.45
1:B:77:PRO:HG3	1:B:83:VAL:HG22	1.99	0.45
1:A:183:ARG:O	1:A:503:TYR:HE2	2.00	0.45
1:B:188:THR:CB	1:B:189:PRO:CD	2.95	0.45
1:B:348:LEU:HB3	1:B:352:ASN:HD21	1.82	0.45
1:B:310:THR:HB	1:B:457:THR:HG21	1.99	0.45
1:B:155:LEU:O	1:B:156:GLU:C	2.55	0.44
1:B:505:THR:HG21	1:B:513:ILE:CD1	2.47	0.44
1:A:78:ARG:HB2	1:A:82:ASP:OD2	2.17	0.44
1:B:13:PRO:HG3	1:B:95:PHE:CE1	2.52	0.44
1:A:295:ILE:HG23	1:A:374:ALA:HB1	1.99	0.44
1:A:155:LEU:O	1:A:156:GLU:C	2.54	0.44
1:A:161:ARG:O	1:A:161:ARG:HG2	2.18	0.44
1:B:62:HIS:H	1:B:62:HIS:CD2	2.35	0.44
1:A:361:GLU:O	1:A:362:PRO:C	2.55	0.44
1:B:324:LYS:HB2	1:B:416:TRP:CD2	2.53	0.44
1:B:79:ASN:HD22	1:B:82:ASP:H	1.60	0.44
1:B:223:PRO:O	1:B:226:MET:HG2	2.17	0.44
1:B:189:PRO:HG2	1:B:270:MET:HE1	2.00	0.44
1:B:309:PRO:HD2	1:B:460:VAL:HB	1.99	0.44
1:A:289:LEU:HD11	1:A:458:PHE:CE2	2.53	0.44
1:B:439:GLN:HA	1:B:500:TRP:CH2	2.52	0.44
1:A:361:GLU:N	1:A:362:PRO:CD	2.80	0.44
1:A:262:VAL:O	2:A:600:FAD:N6A	2.43	0.44
1:A:280:LEU:HB2	1:A:395:LEU:HD22	2.00	0.44
1:B:102:ILE:HG12	1:B:175:SER:HB2	1.98	0.44
1:A:79:ASN:ND2	1:A:82:ASP:N	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:THR:HA	1:B:491:LEU:HD22	2.00	0.43
1:A:284:PRO:O	1:A:350:ARG:HB2	2.17	0.43
1:A:414:ILE:O	1:A:420:GLY:HA3	2.17	0.43
1:A:443:THR:HG21	1:A:469:VAL:CG2	2.46	0.43
1:A:98:TRP:CB	1:A:113:PRO:HB3	2.48	0.43
1:A:13:PRO:HG2	1:A:16:LEU:CD2	2.48	0.43
1:A:297:ARG:CB	1:A:298:PRO:CD	2.90	0.43
2:B:600:FAD:H2'	2:B:600:FAD:H5'2	1.38	0.43
1:B:90:ALA:HB2	1:B:97:LEU:HD21	2.00	0.43
1:B:446:ARG:HB2	1:B:491:LEU:HD21	2.00	0.43
1:A:315:LEU:HD22	1:A:416:TRP:CZ2	2.54	0.43
1:B:230:PRO:O	1:B:233:GLN:HG3	2.19	0.43
1:A:13:PRO:HG3	1:A:95:PHE:CE1	2.54	0.43
1:A:225:THR:HG21	1:A:234:PRO:HG3	2.01	0.43
1:A:526:ARG:HD3	1:A:526:ARG:HA	1.67	0.43
1:B:416:TRP:HB3	1:B:472:VAL:CG2	2.47	0.43
1:B:295:ILE:HG23	1:B:374:ALA:HB1	2.01	0.43
1:B:9:PRO:HG2	1:B:12:LEU:HD23	2.00	0.43
1:B:504:ARG:HD3	1:B:504:ARG:HH11	1.61	0.43
1:B:76:ALA:HA	1:B:77:PRO:HD2	1.85	0.43
1:A:324:LYS:HG3	1:A:416:TRP:CZ2	2.54	0.43
1:B:474:ASN:ND2	1:B:477:ASP:HB2	2.34	0.43
1:B:297:ARG:O	1:B:301:LEU:HB2	2.19	0.42
1:B:446:ARG:HH21	1:B:494:ASP:CG	2.22	0.42
1:A:202:VAL:HG12	1:A:203:VAL:N	2.35	0.42
1:A:141:VAL:HG21	1:A:240:HIS:CE1	2.54	0.42
1:A:258:ASN:HB2	1:A:532:LYS:NZ	2.34	0.42
1:B:272:ASN:OD1	1:B:273:PRO:HD2	2.19	0.42
1:A:80:VAL:CB	1:A:231:GLU:HG2	2.49	0.42
1:B:307:ASN:HB3	1:B:358:TYR:CE1	2.54	0.42
1:A:280:LEU:HD11	1:A:352:ASN:HD22	1.85	0.42
1:A:439:GLN:CA	1:A:500:TRP:CH2	3.02	0.42
1:A:324:LYS:HB2	1:A:416:TRP:CD2	2.54	0.42
1:A:77:PRO:HG3	1:A:83:VAL:HG22	2.01	0.42
1:A:518:ASN:HA	1:A:522:SER:HA	2.01	0.42
1:B:412:LYS:HD3	1:B:412:LYS:O	2.20	0.42
1:B:478:LEU:CD1	1:B:478:LEU:H	2.27	0.42
1:B:446:ARG:HB3	1:B:487:LEU:HD12	2.01	0.42
1:B:79:ASN:HD21	1:B:82:ASP:N	2.17	0.42
1:A:308:VAL:HG13	1:A:460:VAL:O	2.19	0.42
1:B:183:ARG:HG3	1:B:255:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:HIS:O	1:B:507:LEU:C	2.58	0.42
1:A:412:LYS:O	1:A:415:ASP:HB2	2.20	0.42
1:A:417:LEU:HB3	1:A:418:PRO:CD	2.46	0.42
1:A:443:THR:HA	1:A:491:LEU:HD21	2.02	0.42
1:A:367:LEU:CD2	1:B:363:ILE:HD11	2.47	0.42
1:A:549:TRP:HB2	1:A:555:HIS:CE1	2.55	0.41
1:B:281:ILE:HD12	1:B:353:PHE:HD2	1.84	0.41
1:A:425:PHE:CD2	1:A:427:PRO:HD3	2.55	0.41
1:A:76:ALA:HA	1:A:77:PRO:HD2	1.85	0.41
1:B:114:ARG:NH1	1:B:511:ASP:OD2	2.53	0.41
1:B:161:ARG:O	1:B:161:ARG:HG2	2.20	0.41
1:A:307:ASN:HB3	1:A:358:TYR:CE1	2.55	0.41
1:A:312:ARG:CG	1:A:457:THR:HG23	2.43	0.41
1:A:549:TRP:CH2	1:A:558:TRP:HB3	2.55	0.41
1:B:280:LEU:HD11	1:B:282:THR:HG22	2.03	0.41
1:A:131:LEU:HB2	1:A:141:VAL:O	2.19	0.41
2:A:600:FAD:HO3'	2:A:600:FAD:C10	2.29	0.41
1:A:471:ILE:HD13	1:A:487:LEU:HD23	2.02	0.41
1:A:280:LEU:HD11	1:A:282:THR:HG22	2.03	0.41
1:A:315:LEU:CD1	1:A:453:ASP:HB3	2.51	0.41
1:A:125:LYS:HG2	1:A:126:ASN:OD1	2.20	0.41
1:A:79:ASN:ND2	1:A:81:ALA:N	2.69	0.41
1:B:128:ASN:HD22	1:B:128:ASN:HA	1.55	0.41
1:B:468:ILE:HD11	3:B:601:EUG:H93	2.03	0.41
1:A:317:ASP:OD1	1:A:394:VAL:HG11	2.20	0.41
1:A:505:THR:HG21	1:A:513:ILE:HD13	2.03	0.41
1:A:9:PRO:HG2	1:A:12:LEU:HD23	2.03	0.41
1:B:488:MET:HG2	1:B:509:PHE:CE2	2.56	0.41
1:A:223:PRO:O	1:A:226:MET:HG2	2.20	0.41
1:A:319:ALA:HA	1:A:322:GLY:O	2.20	0.41
1:B:398:ARG:O	1:B:401:THR:N	2.54	0.41
1:A:519:TRP:CE3	1:B:211:ARG:HG2	2.56	0.40
1:B:222:ARG:HG3	1:B:224:GLU:OE1	2.21	0.40
1:B:368:TRP:CE3	1:B:368:TRP:HA	2.56	0.40
1:B:315:LEU:HD22	1:B:416:TRP:CH2	2.56	0.40
1:B:505:THR:HG21	1:B:513:ILE:HD13	2.03	0.40
1:A:80:VAL:CG1	1:A:231:GLU:HG2	2.51	0.40
1:A:90:ALA:HB1	1:A:95:PHE:O	2.22	0.40
1:B:424:PHE:CZ	3:B:601:EUG:H6	2.57	0.40
1:B:142:VAL:HG22	1:B:146:VAL:CB	2.51	0.40
1:A:531:LEU:O	1:A:535:VAL:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:600:FAD:H5'2	2:A:600:FAD:H2'	1.35	0.40
1:B:61:HIS:ND1	1:B:422:HIS:ND1	2.70	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	546/560 (98%)	496 (91%)	44 (8%)	6 (1%)	14	41
1	B	546/560 (98%)	491 (90%)	51 (9%)	4 (1%)	22	53
All	All	1092/1120 (98%)	987 (90%)	95 (9%)	10 (1%)	17	46

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	GLY
1	B	420	GLY
1	B	105	ASN
1	A	198	SER
1	A	519	TRP
1	B	418	PRO
1	A	7	PHE
1	A	105	ASN
1	A	418	PRO
1	B	284	PRO

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	462/480 (96%)	429 (93%)	33 (7%)	14	39
1	B	463/480 (96%)	422 (91%)	41 (9%)	9	28
All	All	925/960 (96%)	851 (92%)	74 (8%)	12	34

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	41	SER
1	A	63	VAL
1	A	78	ARG
1	A	79	ASN
1	A	95	PHE
1	A	101	SER
1	A	106	SER
1	A	114	ARG
1	A	116	SER
1	A	128	ASN
1	A	142	VAL
1	A	177	LEU
1	A	198	SER
1	A	211	ARG
1	A	251	ASP
1	A	255	SER
1	A	290	LYS
1	A	314	ILE
1	A	331	THR
1	A	336	ASP
1	A	346	LEU
1	A	350	ARG
1	A	422	HIS
1	A	426	SER
1	A	457	THR
1	A	475	LYS
1	A	503	TYR
1	A	505	THR
1	A	516	THR
1	A	526	ARG
1	A	552	GLN
1	A	554	SER

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Mol	Chain	Res	Type
1	B	7	PHE
1	B	11	THR
1	B	63	VAL
1	B	78	ARG
1	B	79	ASN
1	B	95	PHE
1	B	100	ILE
1	B	106	SER
1	B	114	ARG
1	B	118	SER
1	B	128	ASN
1	B	142	VAL
1	B	177	LEU
1	B	188	THR
1	B	195	MET
1	B	198	SER
1	B	211	ARG
1	B	251	ASP
1	B	255	SER
1	B	283	LEU
1	B	290	LYS
1	B	306	GLN
1	B	314	ILE
1	B	331	THR
1	B	336	ASP
1	B	346	LEU
1	B	350	ARG
1	B	400	LYS
1	B	422	HIS
1	B	426	SER
1	B	457	THR
1	B	467	HIS
1	B	475	LYS
1	B	478	LEU
1	B	502	GLU
1	B	503	TYR
1	B	505	THR
1	B	516	THR
1	B	526	ARG
1	B	552	GLN
1	B	554	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	128	ASN
1	A	158	ASN
1	A	179	ASN
1	A	197	HIS
1	A	277	GLN
1	A	352	ASN
1	A	485	GLN
1	A	520	ASN
1	A	552	GLN
1	A	555	HIS
1	B	79	ASN
1	B	128	ASN
1	B	158	ASN
1	B	179	ASN
1	B	197	HIS
1	B	277	GLN
1	B	352	ASN
1	B	485	GLN
1	B	520	ASN
1	B	552	GLN
1	B	555	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	600	1	51,58,58	1.87	12 (23%)	60,89,89	2.55	22 (36%)
3	EUG	B	601	-	11,11,12	0.58	0	14,14,15	2.70	7 (50%)
3	EUG	A	601	-	11,11,12	0.67	0	14,14,15	3.40	6 (42%)
2	FAD	A	600	1	51,58,58	1.94	12 (23%)	60,89,89	2.37	26 (43%)

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	B	600	1	-	12/30/50/50	0/6/6/6
3	EUG	B	601	-	-	4/4/4/5	0/1/1/1
3	EUG	A	601	-	-	4/4/4/5	0/1/1/1
2	FAD	A	600	1	-	14/30/50/50	0/6/6/6

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C4X-C10	6.72	1.45	1.38
2	B	600	FAD	C4X-C10	6.44	1.45	1.38
2	A	600	FAD	O4B-C1B	5.51	1.48	1.41
2	B	600	FAD	PA-O2A	-4.50	1.34	1.55
2	A	600	FAD	PA-O2A	-4.00	1.36	1.55
2	B	600	FAD	O4B-C1B	3.98	1.46	1.41
2	B	600	FAD	C2B-C1B	-3.70	1.48	1.53
2	A	600	FAD	P-O2P	-3.49	1.38	1.55
2	A	600	FAD	C2B-C1B	-3.36	1.48	1.53
2	B	600	FAD	P-O2P	-3.32	1.39	1.55
2	A	600	FAD	O5'-C5'	2.98	1.56	1.44
2	B	600	FAD	O5'-C5'	2.90	1.55	1.44
2	B	600	FAD	C2-N1	-2.70	1.32	1.38
2	A	600	FAD	C4-N3	2.63	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C2-N1	-2.60	1.33	1.38
2	B	600	FAD	C1'-N10	-2.55	1.45	1.48
2	B	600	FAD	P-O5'	-2.48	1.49	1.59
2	B	600	FAD	C2-N3	2.44	1.43	1.38
2	A	600	FAD	P-O5'	-2.39	1.49	1.59
2	A	600	FAD	C2-N3	2.38	1.42	1.38
2	A	600	FAD	C4-C4X	2.38	1.45	1.41
2	A	600	FAD	C10-N1	2.18	1.36	1.33
2	B	600	FAD	C4-C4X	2.14	1.45	1.41
2	B	600	FAD	C4-N3	2.11	1.36	1.33

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	C4-N3-C2	8.74	122.52	115.14
3	A	601	EUG	O3-C3-C4	8.01	126.18	114.57
2	A	600	FAD	C4-N3-C2	7.56	121.52	115.14
3	A	601	EUG	O3-C3-C2	-6.79	112.43	124.12
2	A	600	FAD	C4X-C4-N3	-6.18	114.98	123.43
2	B	600	FAD	C4X-C4-N3	-6.07	115.13	123.43
3	B	601	EUG	O3-C3-C4	5.22	122.13	114.57
2	B	600	FAD	C6-C5X-N5	-5.15	113.38	119.05
2	A	600	FAD	C6-C5X-N5	-4.90	113.65	119.05
2	B	600	FAD	P-O3P-PA	4.55	148.43	132.83
3	A	601	EUG	C9-O3-C3	4.50	124.32	117.53
2	B	600	FAD	C4X-N5-C5X	-4.46	112.31	116.77
2	A	600	FAD	P-O3P-PA	4.41	147.95	132.83
2	B	600	FAD	C10-C4X-N5	4.41	124.31	121.26
3	B	601	EUG	O3-C3-C2	-4.24	116.82	124.12
2	B	600	FAD	O5B-PA-O1A	-4.21	92.62	109.07
3	B	601	EUG	C9-O3-C3	4.19	123.86	117.53
2	B	600	FAD	C5A-C6A-N6A	4.16	126.68	120.35
2	A	600	FAD	C5'-C4'-C3'	-3.90	104.66	112.20
2	B	600	FAD	C1'-N10-C9A	3.78	121.27	118.29
2	B	600	FAD	C5'-C4'-C3'	-3.75	104.97	112.20
3	A	601	EUG	O4-C4-C3	3.62	128.55	120.09
2	A	600	FAD	O5B-PA-O1A	-3.50	95.41	109.07
2	A	600	FAD	O3B-C3B-C4B	3.35	120.72	111.05
2	A	600	FAD	C4X-N5-C5X	-3.34	113.43	116.77
2	B	600	FAD	O3B-C3B-C4B	3.30	120.59	111.05
2	A	600	FAD	O4B-C1B-C2B	-3.30	102.11	106.93
2	B	600	FAD	C9A-N10-C10	-3.29	117.59	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	EUG	O4-C4-C3	3.15	127.44	120.09
2	B	600	FAD	C4'-C3'-C2'	-3.04	107.03	113.36
2	B	600	FAD	C1'-N10-C10	3.03	121.12	118.41
2	A	600	FAD	C9A-C5X-N5	3.00	127.05	122.36
3	B	601	EUG	C6-C5-C4	-2.96	117.46	120.50
2	B	600	FAD	C2A-N1A-C6A	2.96	123.81	118.75
2	A	600	FAD	C10-C4X-N5	2.94	123.29	121.26
2	B	600	FAD	C9A-C5X-N5	2.93	126.94	122.36
2	A	600	FAD	C5A-C6A-N6A	2.78	124.57	120.35
2	A	600	FAD	C2A-N1A-C6A	2.76	123.48	118.75
2	A	600	FAD	O4'-C4'-C3'	2.73	115.73	109.10
2	A	600	FAD	C4'-C3'-C2'	-2.72	107.70	113.36
2	A	600	FAD	C1'-N10-C9A	2.69	120.41	118.29
3	B	601	EUG	O4-C4-C5	-2.66	112.09	119.33
2	A	600	FAD	C9A-N10-C10	-2.62	118.48	121.91
2	A	600	FAD	O3'-C3'-C2'	-2.54	102.66	108.81
2	B	600	FAD	N3A-C2A-N1A	-2.50	124.77	128.68
2	B	600	FAD	O4'-C4'-C3'	2.49	115.15	109.10
2	A	600	FAD	C1'-N10-C10	2.44	120.59	118.41
2	A	600	FAD	C5A-C6A-N1A	-2.40	114.91	120.35
2	B	600	FAD	C5A-C6A-N1A	-2.36	115.01	120.35
2	A	600	FAD	O2'-C2'-C3'	2.34	114.80	109.10
3	B	601	EUG	C5-C6-C1	2.31	124.25	121.25
2	A	600	FAD	O2A-PA-O1A	2.27	123.47	112.24
2	B	600	FAD	O4B-C4B-C5B	-2.26	101.92	109.37
3	A	601	EUG	O4-C4-C5	-2.25	113.22	119.33
2	B	600	FAD	P-O5'-C5'	2.20	134.59	121.68
3	A	601	EUG	C5-C6-C1	2.17	124.08	121.25
2	A	600	FAD	O4B-C4B-C5B	-2.17	102.24	109.37
2	A	600	FAD	C4-C4X-N5	-2.14	116.15	118.60
2	A	600	FAD	C1'-C2'-C3'	-2.08	103.96	109.79
2	B	600	FAD	C4-C4X-N5	-2.08	116.22	118.60
2	A	600	FAD	O2P-P-O5'	2.00	117.05	107.75

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	FAD	C5B-O5B-PA-O1A
2	B	600	FAD	C5B-O5B-PA-O2A
2	B	600	FAD	C4'-C5'-O5'-P
2	B	600	FAD	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
2	B	600	FAD	C5'-O5'-P-O3P
2	A	600	FAD	C5B-O5B-PA-O1A
2	A	600	FAD	C5B-O5B-PA-O2A
2	A	600	FAD	C4'-C5'-O5'-P
2	A	600	FAD	C5'-O5'-P-O2P
2	A	600	FAD	C5'-O5'-P-O3P
3	A	601	EUG	C4-C3-O3-C9
3	A	601	EUG	C2-C3-O3-C9
3	B	601	EUG	C4-C3-O3-C9
2	A	600	FAD	O4'-C4'-C5'-O5'
2	B	600	FAD	O4B-C4B-C5B-O5B
3	B	601	EUG	C2-C3-O3-C9
2	B	600	FAD	C3'-C4'-C5'-O5'
2	A	600	FAD	C3'-C4'-C5'-O5'
2	A	600	FAD	P-O3P-PA-O1A
2	A	600	FAD	O2'-C2'-C3'-C4'
2	B	600	FAD	P-O3P-PA-O5B
2	A	600	FAD	P-O3P-PA-O5B
2	A	600	FAD	O4B-C4B-C5B-O5B
2	B	600	FAD	C3B-C4B-C5B-O5B
2	A	600	FAD	C3B-C4B-C5B-O5B
3	A	601	EUG	C6-C1-C7-C8
3	A	601	EUG	C2-C1-C7-C8
3	B	601	EUG	C2-C1-C7-C8
3	B	601	EUG	C6-C1-C7-C8
2	B	600	FAD	P-O3P-PA-O1A
2	B	600	FAD	C2'-C3'-C4'-C5'
2	A	600	FAD	C2'-C3'-C4'-C5'
2	B	600	FAD	C5B-O5B-PA-O3P
2	A	600	FAD	C5B-O5B-PA-O3P

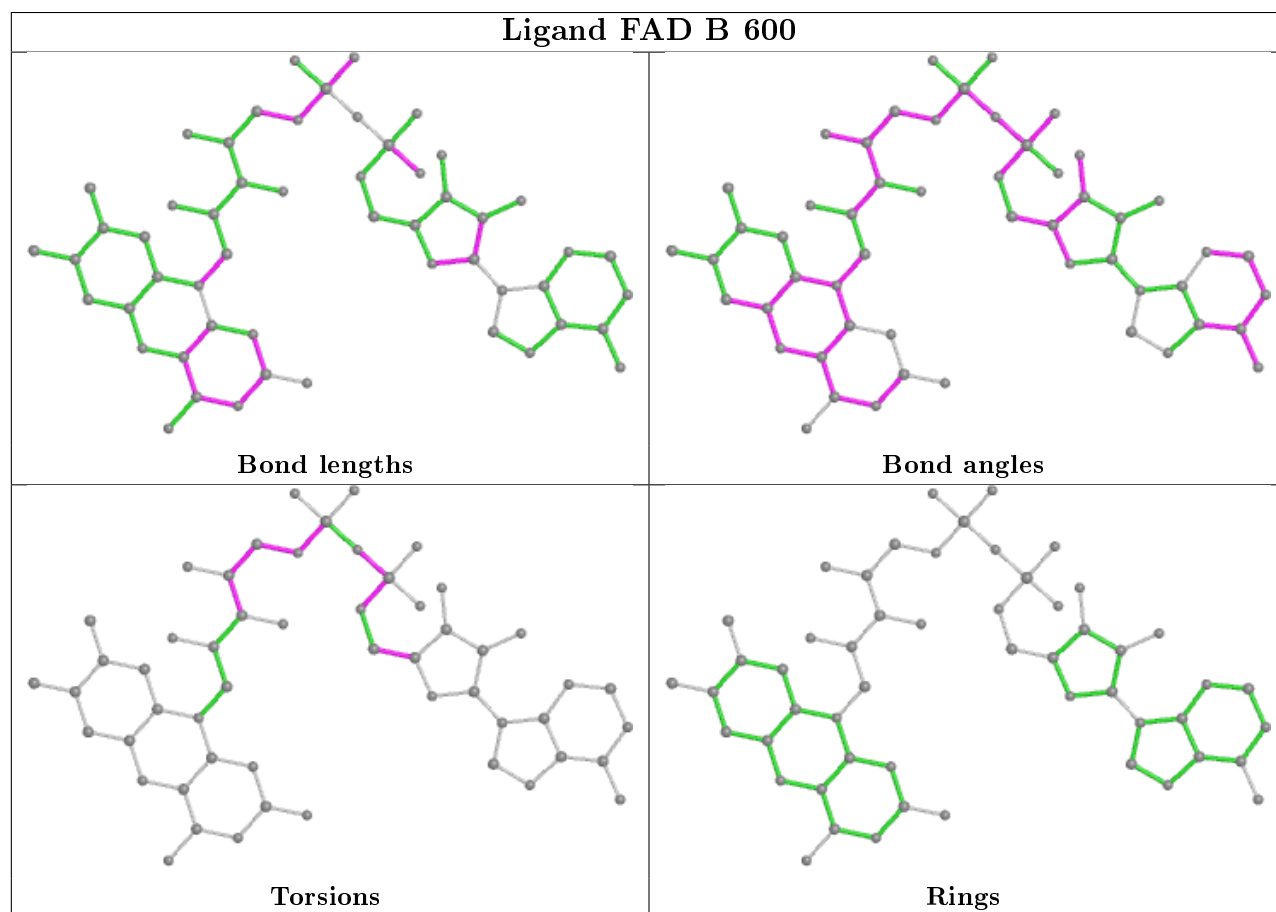
There are no ring outliers.

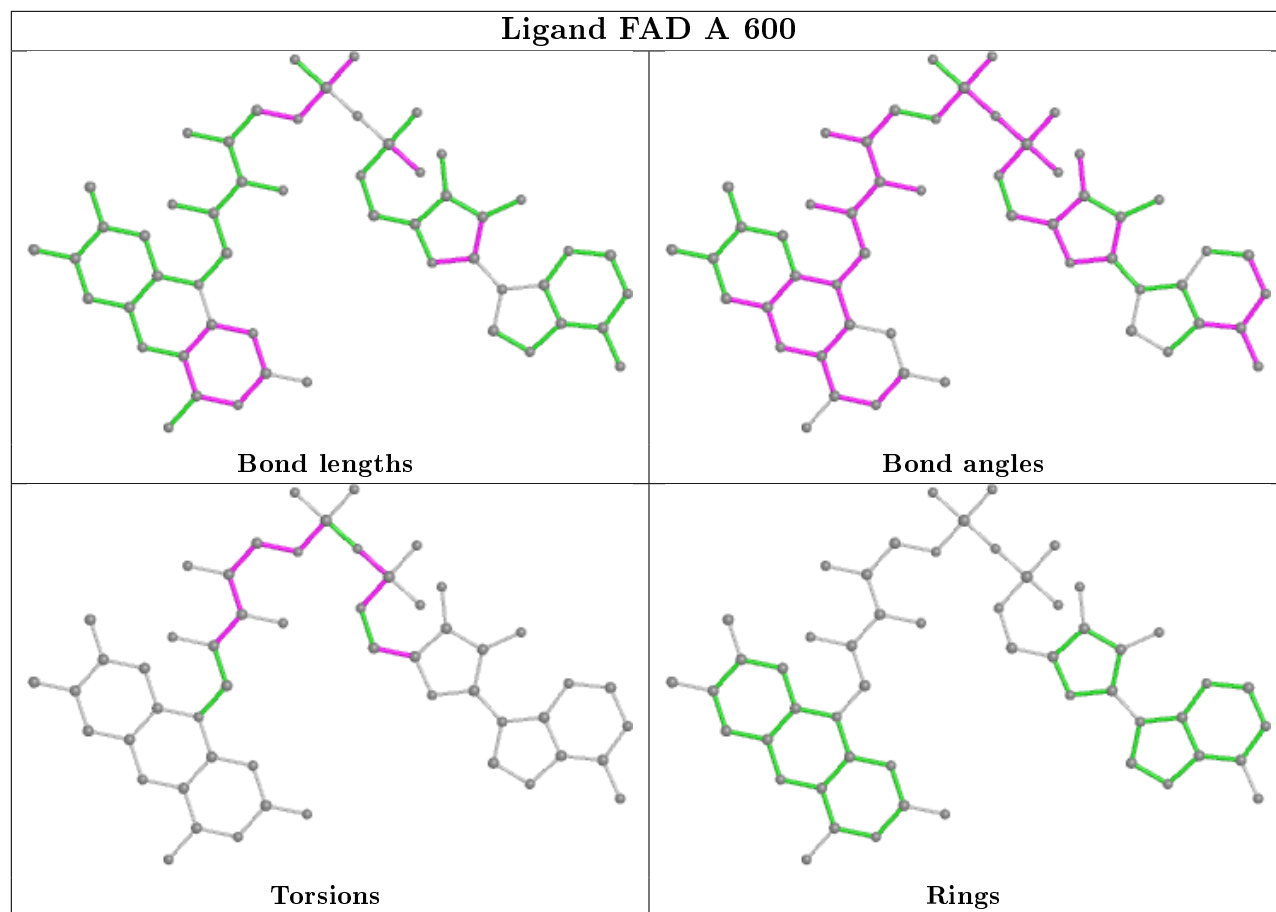
3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	FAD	8	0
3	B	601	EUG	2	0
2	A	600	FAD	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	550/560 (98%)	-0.49	0 100 100	16, 28, 53, 77	0
1	B	550/560 (98%)	-0.46	4 (0%) 87 84	16, 28, 54, 77	0
All	All	1100/1120 (98%)	-0.47	4 (0%) 92 91	16, 28, 54, 77	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	159	ASN	3.8
1	B	6	ALA	3.6
1	B	157	ALA	3.0
1	B	161	ARG	3.0

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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EUG	A	601	11/12	0.91	0.32	34,35,37,37	0

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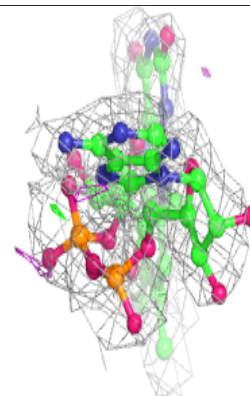
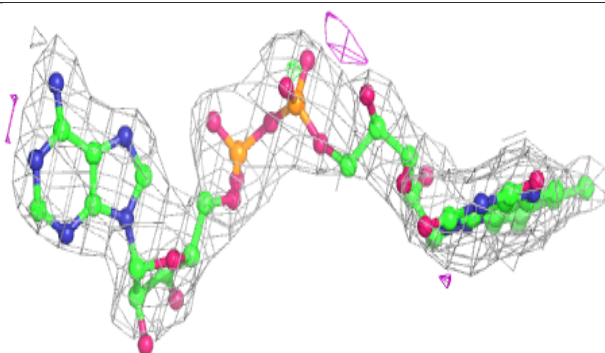
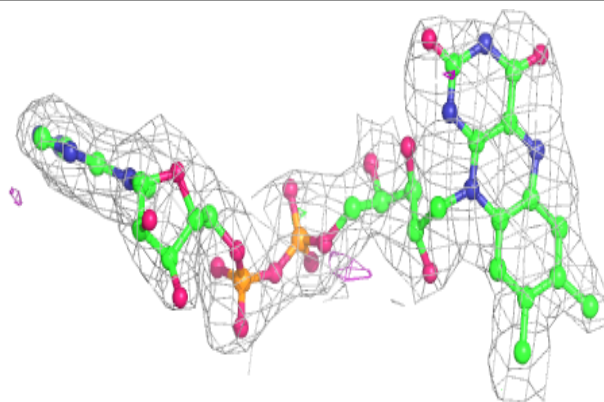
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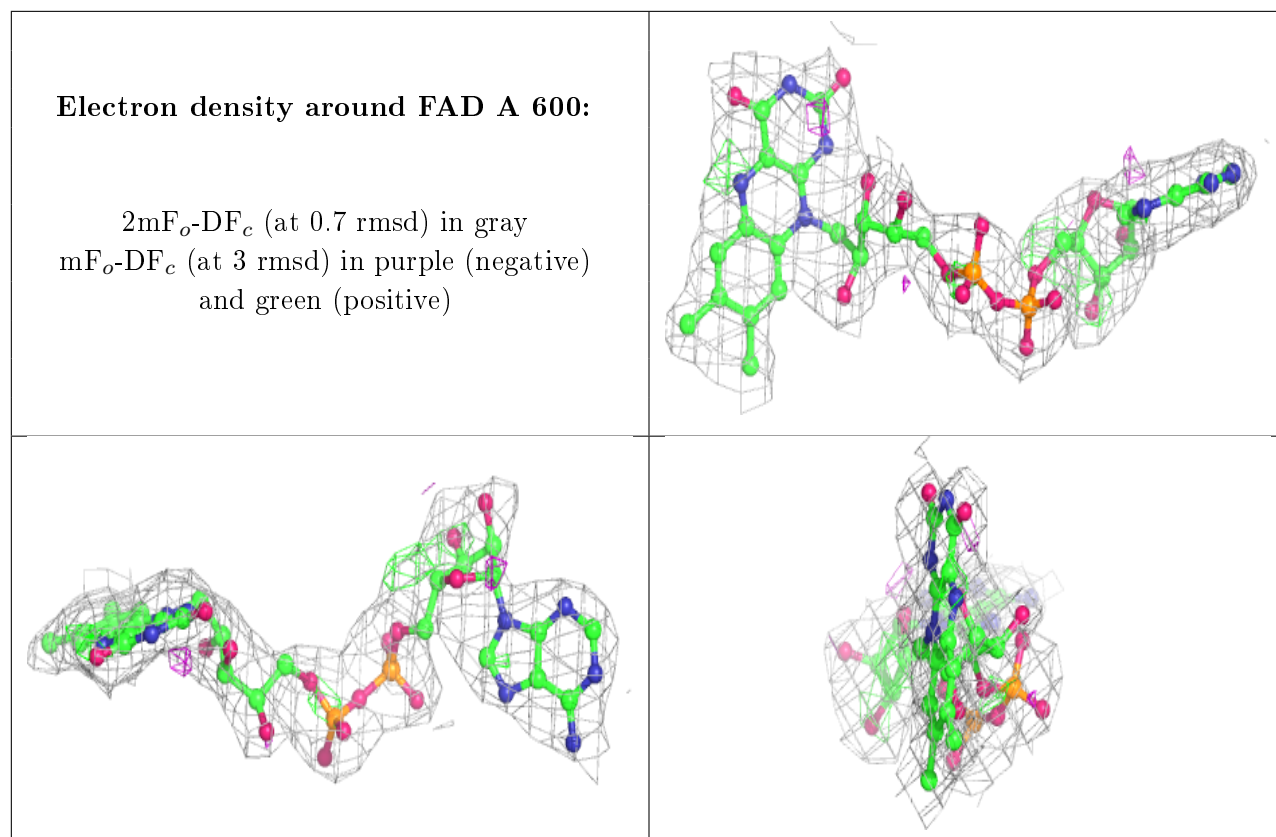
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FAD	B	600	53/53	0.93	0.21	47,51,52,52	0
2	FAD	A	600	53/53	0.93	0.25	47,51,52,52	0
3	EUG	B	601	11/12	0.96	0.20	34,35,37,38	0

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 600:

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.