



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:10 AM UTC

PDB ID : 3LAD / pdb_00003lad
Title : REFINED CRYSTAL STRUCTURE OF LIPOAMIDE DEHYDROGENASE FROM AZOTOBACTER VINELANDII AT 2.2 ANGSTROMS RESOLUTION. A COMPARISON WITH THE STRUCTURE OF GLUTATHIONE REDUCTASE
Authors : Mattevi, A.; Schierbeek, A.J.; Hol, W.G.J.
Deposited on : 1991-12-11
Resolution : 2.20 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)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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

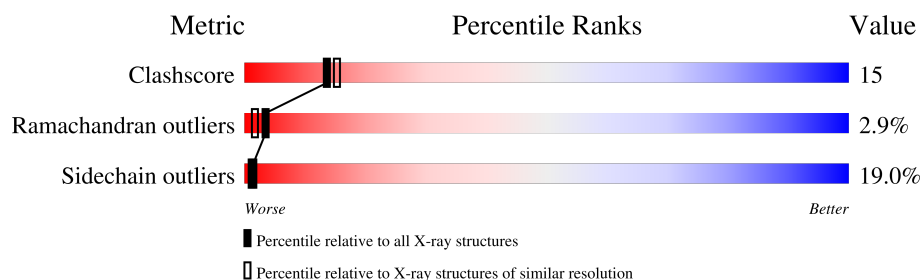
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 was not executed.

Mol	Chain	Length	Quality of chain
1	A	476	45% 36% 15% ..
1	B	476	53% 31% 13% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7411 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 DIHYDROLIPOAMIDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3427	2174	585	657	11			
1	B	472	Total	C	N	O	S	0	0	0
			3427	2174	585	657	11			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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 water.

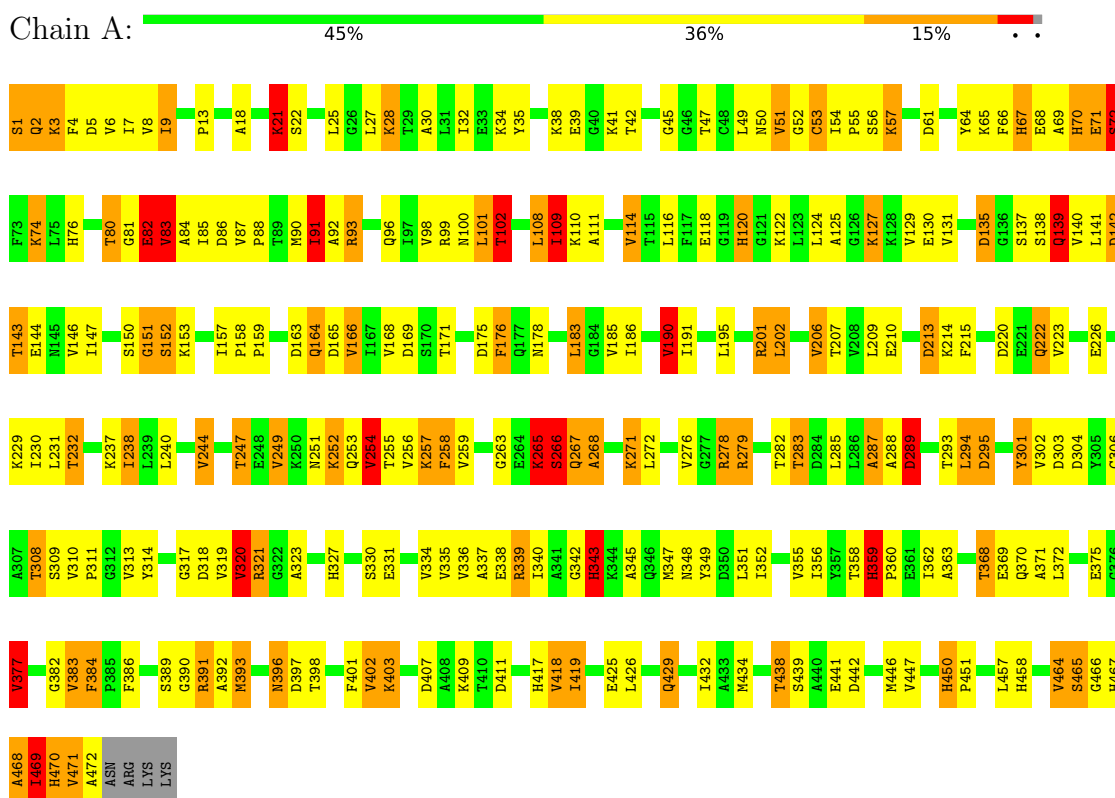
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	212	Total 212	O 212	0	0
3	B	239	Total 239	O 239	0	0

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. 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. 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.

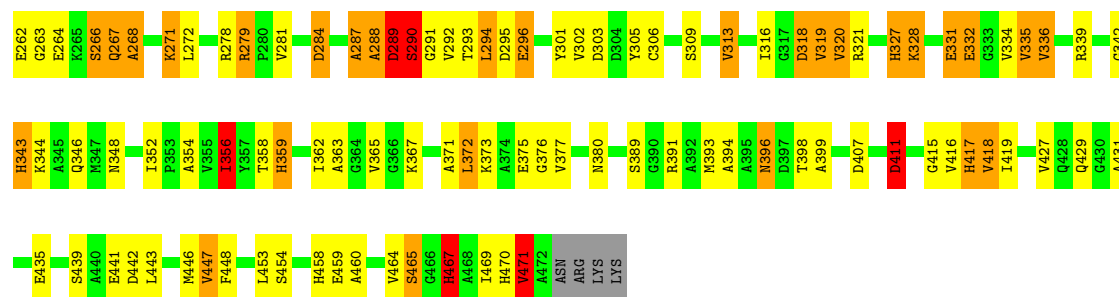
Note EDS was not executed.

• Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE



• Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.13Å 83.86Å 191.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GROMOS, TNT, X-PLOR	Depositor
R, R_{free}	0.192 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7411	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.36	32/3478 (0.9%)	2.20	164/4717 (3.5%)
1	B	1.34	34/3478 (1.0%)	2.23	159/4717 (3.4%)
All	All	1.35	66/6956 (0.9%)	2.22	323/9434 (3.4%)

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	2
1	B	0	2
All	All	0	4

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	468	ALA	N-CA	21.17	1.73	1.46
1	B	356	ILE	CA-CB	11.84	1.69	1.54
1	A	84	ALA	N-CA	11.49	1.59	1.45
1	A	418	VAL	CA-CB	10.29	1.68	1.54
1	A	352	ILE	CA-CB	8.80	1.60	1.54
1	A	91	ILE	CA-CB	8.46	1.65	1.54
1	A	377	VAL	CA-CB	7.78	1.63	1.54
1	B	157	ILE	CA-CB	7.55	1.64	1.54
1	A	238	ILE	CA-CB	7.42	1.62	1.54
1	A	327	HIS	CG-ND1	-7.08	1.30	1.38
1	A	76	HIS	CD2-NE2	-7.07	1.30	1.37
1	A	206	VAL	CA-CB	7.07	1.64	1.54
1	B	83	VAL	CA-CB	6.99	1.63	1.54
1	B	32	ILE	CA-CB	6.88	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	HIS	CD2-NE2	-6.85	1.30	1.37
1	A	327	HIS	CD2-NE2	-6.69	1.30	1.37
1	B	417	HIS	CD2-NE2	-6.65	1.30	1.37
1	A	458	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	157	ILE	CA-CB	6.56	1.62	1.54
1	A	470	HIS	CD2-NE2	-6.51	1.30	1.37
1	B	319	VAL	CA-CB	6.46	1.62	1.54
1	B	418	VAL	CA-CB	6.35	1.63	1.54
1	B	343	HIS	CD2-NE2	-6.34	1.30	1.37
1	A	8	VAL	CA-CB	6.33	1.61	1.54
1	A	83	VAL	CA-C	6.30	1.60	1.52
1	A	419	ILE	CA-CB	6.27	1.61	1.54
1	B	67	HIS	CD2-NE2	-6.22	1.31	1.37
1	B	336	VAL	CA-CB	6.22	1.61	1.54
1	B	417	HIS	CG-ND1	-6.21	1.31	1.38
1	B	313	VAL	CA-CB	6.15	1.61	1.54
1	B	266	SER	CA-CB	-6.13	1.44	1.53
1	B	70	HIS	CD2-NE2	-6.11	1.31	1.37
1	A	83	VAL	C-N	6.10	1.41	1.33
1	B	51	VAL	CA-CB	6.08	1.62	1.54
1	B	76	HIS	CD2-NE2	-6.03	1.31	1.37
1	B	78	ILE	CA-CB	6.01	1.61	1.54
1	A	139	GLN	CA-CB	-5.98	1.43	1.53
1	B	120	HIS	CD2-NE2	-5.97	1.31	1.37
1	B	70	HIS	CG-ND1	-5.96	1.31	1.38
1	B	359	HIS	CD2-NE2	-5.94	1.31	1.37
1	B	67	HIS	CG-ND1	-5.93	1.31	1.38
1	A	343	HIS	CD2-NE2	-5.88	1.31	1.37
1	B	458	HIS	CD2-NE2	-5.88	1.31	1.37
1	A	244	VAL	CA-CB	5.81	1.61	1.54
1	B	249	VAL	CA-CB	5.81	1.61	1.54
1	A	109	ILE	CA-CB	5.80	1.62	1.54
1	A	67	HIS	CD2-NE2	-5.78	1.31	1.37
1	A	450	HIS	CD2-NE2	-5.78	1.31	1.37
1	A	190	VAL	CA-CB	5.76	1.62	1.54
1	B	20	ILE	CA-CB	5.74	1.61	1.54
1	B	471	VAL	CA-CB	5.74	1.62	1.54
1	A	467	HIS	CD2-NE2	-5.74	1.31	1.37
1	A	417	HIS	CG-ND1	-5.72	1.31	1.38
1	A	276	VAL	CA-CB	5.69	1.62	1.54
1	B	327	HIS	CD2-NE2	-5.61	1.31	1.37
1	A	417	HIS	CD2-NE2	-5.43	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	447	VAL	CA-CB	5.41	1.59	1.53
1	A	450	HIS	CG-ND1	-5.31	1.32	1.38
1	B	109	ILE	CA-CB	5.18	1.61	1.54
1	B	464	VAL	CA-CB	5.16	1.60	1.54
1	B	327	HIS	CG-ND1	-5.15	1.32	1.38
1	A	120	HIS	CD2-NE2	-5.12	1.32	1.37
1	B	120	HIS	CG-ND1	-5.12	1.32	1.38
1	B	206	VAL	CA-CB	5.11	1.60	1.54
1	B	216	LEU	CA-CB	5.11	1.57	1.52
1	B	419	ILE	CA-CB	5.00	1.60	1.54

All (323) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	ASP	CA-CB-CG	16.70	129.30	112.60
1	B	411	ASP	CA-CB-CG	13.52	126.12	112.60
1	B	290	SER	N-CA-C	-12.33	85.36	108.17
1	B	303	ASP	CA-CB-CG	11.51	124.11	112.60
1	A	407	ASP	CA-CB-CG	11.37	123.97	112.60
1	B	289	ASP	N-CA-C	11.11	134.46	110.80
1	A	370	GLN	OE1-CD-NE2	-9.86	112.75	122.60
1	B	67	HIS	ND1-CG-CD2	9.80	115.90	106.10
1	B	176	PHE	CA-CB-CG	9.78	123.58	113.80
1	B	359	HIS	O-C-N	-9.69	113.38	121.23
1	B	234	GLN	OE1-CD-NE2	-9.66	112.94	122.60
1	B	178	ASN	OD1-CG-ND2	-9.53	113.07	122.60
1	A	289	ASP	CA-CB-CG	-9.38	103.22	112.60
1	B	72	SER	N-CA-C	9.31	126.07	112.94
1	A	359	HIS	ND1-CG-CD2	9.25	115.35	106.10
1	A	142	ASP	CA-CB-CG	8.74	121.34	112.60
1	B	87	VAL	O-C-N	-8.74	114.83	120.42
1	A	356	ILE	N-CA-C	-8.73	95.95	108.17
1	A	396	ASN	OD1-CG-ND2	-8.53	114.07	122.60
1	A	467	HIS	CA-C-N	8.49	135.17	123.11
1	A	467	HIS	C-N-CA	8.49	135.17	123.11
1	B	419	ILE	N-CA-C	-8.20	96.63	108.11
1	B	213	ASP	CA-CB-CG	8.12	120.72	112.60
1	B	359	HIS	ND1-CG-CD2	8.09	114.19	106.10
1	B	70	HIS	ND1-CG-CD2	8.09	114.19	106.10
1	A	163	ASP	CA-CB-CG	8.05	120.65	112.60
1	A	327	HIS	ND1-CG-CD2	7.97	114.07	106.10
1	A	359	HIS	CA-CB-CG	7.91	121.71	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	VAL	N-CA-CB	-7.86	98.27	111.23
1	A	368	THR	N-CA-CB	-7.83	99.16	110.36
1	B	164	GLN	OE1-CD-NE2	-7.82	114.78	122.60
1	B	301	TYR	O-C-N	7.81	132.53	122.93
1	B	467	HIS	CA-CB-CG	7.79	121.59	113.80
1	A	458	HIS	ND1-CG-CD2	7.78	113.88	106.10
1	B	258	PHE	CA-CB-CG	7.78	121.58	113.80
1	A	120	HIS	ND1-CG-CD2	7.77	113.87	106.10
1	B	120	HIS	ND1-CG-CD2	7.74	113.84	106.10
1	B	411	ASP	N-CA-C	7.69	127.18	110.80
1	B	178	ASN	CB-CG-ND2	7.65	127.87	116.40
1	B	396	ASN	OD1-CG-ND2	-7.60	115.00	122.60
1	A	396	ASN	CB-CG-ND2	7.58	127.78	116.40
1	B	250	LYS	N-CA-C	-7.58	96.90	108.96
1	B	287	ALA	O-C-N	-7.57	113.82	122.68
1	A	86	ASP	CA-C-N	7.55	125.00	120.24
1	A	86	ASP	C-N-CA	7.55	125.00	120.24
1	B	171	THR	N-CA-C	7.54	119.50	111.28
1	B	51	VAL	N-CA-CB	-7.54	98.80	111.23
1	B	101	LEU	N-CA-C	7.52	119.56	111.36
1	B	100	ASN	OD1-CG-ND2	-7.47	115.13	122.60
1	B	67	HIS	CG-CD2-NE2	-7.45	99.75	107.20
1	A	158	PRO	N-CA-C	7.45	119.78	110.70
1	A	343	HIS	ND1-CG-CD2	7.41	113.51	106.10
1	B	178	ASN	CA-CB-CG	7.31	119.91	112.60
1	A	96	GLN	OE1-CD-NE2	-7.29	115.31	122.60
1	A	2	GLN	N-CA-C	7.29	126.33	110.80
1	A	321	ARG	CA-CB-CG	7.28	128.66	114.10
1	B	70	HIS	CA-CB-CG	-7.28	106.52	113.80
1	A	320	VAL	CA-CB-CG2	-7.25	98.07	110.40
1	A	191	ILE	CB-CA-C	-7.21	102.65	111.88
1	B	460	ALA	N-CA-C	-7.19	103.37	111.07
1	B	267	GLN	CA-C-O	7.17	128.94	120.70
1	B	239	LEU	N-CA-C	-7.13	97.11	108.73
1	B	76	HIS	ND1-CG-CD2	7.12	113.22	106.10
1	A	304	ASP	CA-CB-CG	7.11	119.71	112.60
1	B	318	ASP	N-CA-C	7.11	121.41	112.87
1	B	111	ALA	CA-C-O	7.08	128.13	120.20
1	A	135	ASP	CA-CB-CG	7.08	119.68	112.60
1	A	151	GLY	N-CA-C	7.04	122.17	112.52
1	B	416	VAL	N-CA-C	-7.04	97.29	107.78
1	A	249	VAL	N-CA-C	-6.99	97.54	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	GLN	CG-CD-NE2	6.96	126.84	116.40
1	A	429	GLN	OE1-CD-NE2	-6.91	115.69	122.60
1	A	348	ASN	OD1-CG-ND2	-6.90	115.70	122.60
1	B	328	LYS	N-CA-C	-6.88	103.47	110.97
1	A	336	VAL	CA-C-O	-6.88	113.42	121.05
1	A	153	LYS	CA-C-O	-6.87	114.73	120.71
1	B	236	LEU	N-CA-C	-6.84	98.09	108.96
1	B	415	GLY	O-C-N	-6.84	117.27	123.36
1	A	183	LEU	CA-C-N	6.84	126.90	122.18
1	A	183	LEU	C-N-CA	6.84	126.90	122.18
1	A	458	HIS	CG-CD2-NE2	-6.81	100.39	107.20
1	B	51	VAL	CB-CA-C	6.78	122.40	111.29
1	B	169	ASP	CA-CB-CG	6.77	119.37	112.60
1	B	234	GLN	CB-CG-CD	6.75	124.07	112.60
1	A	2	GLN	OE1-CD-NE2	-6.74	115.86	122.60
1	B	199	TRP	CG-CD2-CE3	6.74	140.64	133.90
1	B	284	ASP	CA-CB-CG	6.74	119.34	112.60
1	A	65	LYS	N-CA-C	-6.73	103.87	111.14
1	A	76	HIS	ND1-CG-CD2	6.68	112.78	106.10
1	B	167	ILE	CB-CG1-CD1	-6.67	99.79	113.80
1	A	359	HIS	CG-CD2-NE2	-6.66	100.54	107.20
1	A	102	THR	N-CA-CB	-6.66	100.36	110.01
1	B	173	ALA	N-CA-C	6.65	122.35	111.37
1	A	417	HIS	ND1-CG-CD2	6.64	112.74	106.10
1	B	128	LYS	N-CA-C	-6.63	100.71	110.52
1	A	1	SER	CA-C-N	6.62	134.19	121.54
1	A	1	SER	C-N-CA	6.62	134.19	121.54
1	A	464	VAL	N-CA-C	-6.58	104.07	110.72
1	B	166	VAL	N-CA-C	-6.58	104.61	111.58
1	A	470	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	A	362	ILE	O-C-N	-6.57	116.66	123.03
1	A	438	THR	N-CA-C	6.57	118.78	110.24
1	B	87	VAL	CA-C-O	-6.56	114.30	118.69
1	B	289	ASP	CA-CB-CG	6.53	119.13	112.60
1	A	318	ASP	CA-CB-CG	6.53	119.13	112.60
1	A	327	HIS	CA-CB-CG	6.53	120.33	113.80
1	B	168	VAL	N-CA-CB	-6.51	100.31	112.36
1	B	201	ARG	CB-CG-CD	6.51	126.27	111.30
1	B	23	ALA	N-CA-C	-6.44	104.19	111.14
1	A	343	HIS	CA-CB-CG	6.43	120.23	113.80
1	B	417	HIS	ND1-CG-CD2	6.43	112.53	106.10
1	A	339	ARG	CA-CB-CG	6.42	126.94	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	VAL	CA-C-N	6.42	126.64	119.32
1	A	310	VAL	C-N-CA	6.42	126.64	119.32
1	A	67	HIS	ND1-CG-CD2	6.41	112.51	106.10
1	B	145	ASN	CA-CB-CG	6.41	119.01	112.60
1	B	342	GLY	O-C-N	6.40	131.02	122.70
1	A	258	PHE	CA-CB-CG	6.37	120.17	113.80
1	B	290	SER	CA-CB-OG	6.37	123.83	111.10
1	A	65	LYS	CA-CB-CG	6.36	126.82	114.10
1	A	147	ILE	O-C-N	-6.33	116.22	122.99
1	A	223	VAL	CA-C-O	-6.32	114.47	121.17
1	B	287	ALA	CA-C-O	-6.31	114.50	121.89
1	A	111	ALA	O-C-N	-6.31	115.57	122.07
1	A	267	GLN	O-C-N	6.30	131.38	123.01
1	A	267	GLN	CA-C-O	6.29	127.93	120.70
1	A	87	VAL	CG1-CB-CG2	-6.28	96.99	110.80
1	A	295	ASP	CA-CB-CG	6.27	118.87	112.60
1	B	71	GLU	N-CA-C	6.25	119.03	111.40
1	A	169	ASP	CA-CB-CG	6.25	118.85	112.60
1	B	327	HIS	ND1-CG-CD2	6.22	112.32	106.10
1	A	150	SER	O-C-N	-6.20	114.12	122.43
1	A	360	PRO	N-CA-C	-6.17	100.78	111.32
1	A	5	ASP	N-CA-C	-6.14	105.81	113.55
1	A	41	LYS	N-CA-C	6.14	118.45	110.53
1	A	176	PHE	CA-CB-CG	6.12	119.92	113.80
1	A	144	GLU	CB-CG-CD	6.12	123.00	112.60
1	A	397	ASP	CA-CB-CG	6.11	118.71	112.60
1	B	458	HIS	ND1-CG-CD2	6.11	112.21	106.10
1	B	71	GLU	CB-CA-C	-6.09	100.55	110.79
1	A	120	HIS	CG-CD2-NE2	-6.09	101.11	107.20
1	A	470	HIS	CA-CB-CG	-6.09	107.71	113.80
1	A	392	ALA	CA-C-N	6.05	128.31	120.44
1	A	392	ALA	C-N-CA	6.05	128.31	120.44
1	A	76	HIS	CG-CD2-NE2	-6.05	101.15	107.20
1	B	240	LEU	N-CA-C	6.04	120.65	113.16
1	B	399	ALA	N-CA-C	6.04	119.36	109.76
1	B	234	GLN	CG-CD-NE2	6.02	125.43	116.40
1	A	254	VAL	CB-CA-C	-6.01	102.83	111.19
1	A	384	PHE	CA-C-N	6.01	126.51	120.14
1	A	384	PHE	C-N-CA	6.01	126.51	120.14
1	A	450	HIS	ND1-CG-CD2	6.00	112.11	106.10
1	A	210	GLU	N-CA-C	6.00	118.19	108.41
1	B	335	VAL	O-C-N	5.97	127.76	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	296	GLU	CB-CG-CD	5.96	122.73	112.60
1	A	337	ALA	N-CA-C	5.95	118.55	111.71
1	B	346	GLN	CB-CG-CD	5.94	122.70	112.60
1	A	255	THR	N-CA-C	-5.93	99.61	109.46
1	B	380	ASN	CA-CB-CG	5.92	118.52	112.60
1	B	327	HIS	CG-CD2-NE2	-5.91	101.29	107.20
1	B	460	ALA	O-C-N	-5.91	115.98	122.07
1	B	448	PHE	CA-C-O	-5.90	113.94	120.38
1	B	70	HIS	CG-CD2-NE2	-5.89	101.31	107.20
1	B	279	ARG	CA-C-O	-5.89	114.92	120.34
1	B	19	ALA	N-CA-C	5.89	117.37	111.07
1	B	73	PHE	CA-CB-CG	-5.88	107.92	113.80
1	A	202	LEU	N-CA-C	-5.86	106.13	113.28
1	A	438	THR	CA-CB-OG1	-5.84	100.84	109.60
1	A	465	SER	N-CA-CB	-5.84	102.50	110.56
1	B	108	LEU	CA-C-O	-5.84	114.32	120.63
1	B	147	ILE	CB-CA-C	-5.84	103.75	110.41
1	B	346	GLN	OE1-CD-NE2	-5.84	116.76	122.60
1	A	320	VAL	N-CA-CB	-5.83	101.61	111.23
1	B	157	ILE	CA-C-N	5.83	126.39	120.38
1	B	157	ILE	C-N-CA	5.83	126.39	120.38
1	B	190	VAL	N-CA-CB	-5.82	104.05	110.51
1	A	114	VAL	CA-C-O	-5.82	113.63	121.02
1	A	294	LEU	CA-C-O	5.81	128.13	121.28
1	B	50	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	A	70	HIS	CA-CB-CG	-5.80	108.00	113.80
1	B	343	HIS	ND1-CG-CD2	5.79	111.89	106.10
1	A	320	VAL	CA-CB-CG1	5.79	120.24	110.40
1	B	251	ASN	CA-CB-CG	5.78	118.38	112.60
1	A	164	GLN	CA-CB-CG	5.77	125.64	114.10
1	B	70	HIS	CA-C-O	-5.77	114.94	121.00
1	B	313	VAL	N-CA-C	-5.76	100.11	108.17
1	B	459	GLU	N-CA-C	5.74	117.62	111.36
1	A	468	ALA	N-CA-CB	5.73	119.99	110.47
1	B	471	VAL	CB-CA-C	5.73	120.69	111.29
1	A	127	LYS	N-CA-C	5.73	123.00	110.80
1	A	53	CYS	N-CA-C	5.72	122.98	110.80
1	B	254	VAL	CB-CA-C	-5.71	102.18	110.63
1	A	93	ARG	NE-CZ-NH2	-5.69	114.08	119.20
1	A	470	HIS	CB-CG-ND1	5.69	131.23	122.70
1	A	368	THR	O-C-N	-5.68	116.31	122.79
1	A	201	ARG	CA-CB-CG	-5.68	102.73	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	120	HIS	CG-CD2-NE2	-5.67	101.53	107.20
1	A	417	HIS	CG-CD2-NE2	-5.67	101.53	107.20
1	B	251	ASN	N-CA-C	5.67	122.87	110.80
1	A	152	SER	CA-CB-OG	5.66	122.42	111.10
1	A	360	PRO	O-C-N	5.66	130.19	123.06
1	B	106	ALA	CA-C-O	-5.65	114.57	120.55
1	B	352	ILE	N-CA-C	-5.64	101.30	107.73
1	A	185	VAL	N-CA-C	-5.64	99.37	107.78
1	B	221	GLU	O-C-N	-5.64	116.22	122.09
1	A	9	ILE	N-CA-C	5.63	115.44	106.88
1	A	386	PHE	CA-CB-CG	-5.63	108.17	113.80
1	A	90	MET	N-CA-C	-5.62	105.23	111.36
1	B	398	THR	N-CA-C	5.61	119.82	112.92
1	B	288	ALA	CA-C-N	5.58	132.20	121.54
1	B	288	ALA	C-N-CA	5.58	132.20	121.54
1	A	28	LYS	N-CA-C	-5.58	101.12	109.15
1	A	206	VAL	N-CA-C	5.57	116.50	108.48
1	B	469	ILE	CB-CA-C	-5.57	104.78	112.24
1	B	194	GLU	CA-CB-CG	-5.55	102.99	114.10
1	A	61	ASP	CA-C-O	-5.55	114.61	120.55
1	A	232	THR	N-CA-C	-5.55	105.31	111.36
1	B	439	SER	N-CA-C	-5.55	101.98	110.14
1	A	419	ILE	O-C-N	-5.54	115.66	122.97
1	A	340	ILE	N-CA-C	-5.52	104.94	110.30
1	A	96	GLN	CG-CD-NE2	5.51	124.66	116.40
1	B	320	VAL	N-CA-CB	-5.51	100.51	111.91
1	A	164	GLN	OE1-CD-NE2	-5.50	117.10	122.60
1	A	370	GLN	CA-CB-CG	5.50	125.09	114.10
1	B	29	THR	N-CA-C	5.46	118.14	109.24
1	B	220	ASP	CA-C-N	5.46	127.91	120.54
1	B	220	ASP	C-N-CA	5.46	127.91	120.54
1	A	398	THR	N-CA-C	5.46	119.92	112.88
1	A	343	HIS	CG-CD2-NE2	-5.44	101.76	107.20
1	A	383	VAL	O-C-N	-5.44	117.30	123.18
1	B	138	SER	N-CA-C	-5.44	99.81	109.06
1	B	160	ALA	CA-C-N	5.42	125.59	119.90
1	B	160	ALA	C-N-CA	5.42	125.59	119.90
1	A	401	PHE	CA-CB-CG	5.41	119.21	113.80
1	A	467	HIS	N-CA-C	5.41	119.73	108.53
1	B	431	ALA	CA-C-N	5.40	127.36	120.56
1	B	431	ALA	C-N-CA	5.40	127.36	120.56
1	A	100	ASN	O-C-N	-5.40	116.40	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	THR	CB-CA-C	5.40	119.35	110.88
1	A	82	GLU	O-C-N	5.39	129.76	122.59
1	B	336	VAL	N-CA-C	5.38	115.59	110.42
1	A	215	PHE	CA-C-O	5.38	126.83	120.69
1	B	365	VAL	N-CA-C	-5.38	100.09	108.81
1	B	254	VAL	CA-C-O	-5.37	114.76	120.39
1	A	50	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	A	18	ALA	CB-CA-C	-5.36	101.90	110.79
1	B	42	THR	CA-CB-OG1	-5.35	101.57	109.60
1	B	278	ARG	CD-NE-CZ	-5.34	116.92	124.40
1	A	135	ASP	N-CA-C	5.34	119.10	112.59
1	B	180	PRO	O-C-N	-5.33	116.50	123.06
1	B	155	VAL	CA-CB-CG2	-5.33	101.34	110.40
1	B	194	GLU	CB-CA-C	-5.33	101.80	110.85
1	A	67	HIS	CB-CG-CD2	-5.32	124.29	131.20
1	A	303	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	402	VAL	CG1-CB-CG2	-5.32	99.10	110.80
1	B	38	LYS	N-CA-C	5.32	119.25	112.87
1	A	137	SER	N-CA-C	-5.31	101.12	109.25
1	A	391	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	B	155	VAL	CA-CB-CG1	5.30	119.41	110.40
1	B	20	ILE	N-CA-C	-5.30	105.55	110.53
1	B	371	ALA	N-CA-C	-5.28	105.19	111.69
1	B	222	GLN	CA-C-N	5.28	127.31	120.56
1	B	222	GLN	C-N-CA	5.28	127.31	120.56
1	A	190	VAL	CG1-CB-CG2	-5.26	99.22	110.80
1	B	359	HIS	CA-C-O	-5.26	115.87	119.29
1	B	335	VAL	CG1-CB-CG2	-5.26	99.23	110.80
1	A	403	LYS	CG-CD-CE	-5.26	99.21	111.30
1	B	262	GLU	CA-CB-CG	5.26	124.61	114.10
1	B	348	ASN	CA-C-O	5.25	126.20	120.58
1	B	359	HIS	CG-CD2-NE2	-5.25	101.95	107.20
1	B	29	THR	O-C-N	-5.24	117.34	123.27
1	A	401	PHE	N-CA-C	5.24	115.45	108.38
1	B	71	GLU	CA-CB-CG	5.24	124.58	114.10
1	A	266	SER	CA-C-O	5.24	126.94	120.92
1	B	82	GLU	N-CA-C	-5.23	100.77	109.46
1	B	98	VAL	CA-C-N	5.23	127.24	120.44
1	B	98	VAL	C-N-CA	5.23	127.24	120.44
1	B	70	HIS	CB-CG-CD2	-5.23	124.40	131.20
1	A	171	THR	OG1-CB-CG2	5.22	119.73	109.30
1	A	345	ALA	N-CA-C	5.22	116.45	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	HIS	CB-CG-CD2	-5.22	124.42	131.20
1	A	393	MET	N-CA-CB	-5.21	102.45	110.01
1	A	278	ARG	NE-CZ-NH2	-5.21	114.51	119.20
1	B	206	VAL	N-CA-C	5.21	115.40	108.11
1	B	67	HIS	O-C-N	-5.19	116.14	122.22
1	A	336	VAL	N-CA-C	-5.19	105.65	110.53
1	A	21	LYS	CG-CD-CE	5.18	123.22	111.30
1	A	359	HIS	CA-C-O	-5.17	113.08	120.16
1	B	112	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	B	139	GLN	O-C-N	-5.16	117.09	123.44
1	A	279	ARG	CA-CB-CG	5.16	124.42	114.10
1	B	250	LYS	CA-C-N	5.16	131.40	121.54
1	B	250	LYS	C-N-CA	5.16	131.40	121.54
1	A	65	LYS	CG-CD-CE	-5.14	99.47	111.30
1	A	229	LYS	CA-C-O	5.14	126.00	120.70
1	A	166	VAL	CG1-CB-CG2	-5.13	99.50	110.80
1	A	283	THR	N-CA-C	5.13	121.73	110.80
1	B	263	GLY	N-CA-C	-5.12	101.03	113.18
1	B	179	VAL	CB-CA-C	-5.12	105.36	110.89
1	A	285	LEU	CA-CB-CG	5.11	134.20	116.30
1	B	278	ARG	N-CA-C	-5.09	101.80	109.85
1	B	235	GLY	CA-C-O	5.09	125.62	119.82
1	B	199	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	B	165	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	448	PHE	N-CA-C	-5.08	100.88	109.07
1	A	2	GLN	CA-C-N	5.08	131.25	121.54
1	A	2	GLN	C-N-CA	5.08	131.25	121.54
1	B	179	VAL	CA-C-N	5.08	124.98	119.85
1	B	179	VAL	C-N-CA	5.08	124.98	119.85
1	B	294	LEU	O-C-N	-5.08	116.76	123.16
1	A	265	LYS	CB-CG-CD	-5.07	99.64	111.30
1	A	347	MET	CA-CB-CG	5.07	124.24	114.10
1	B	7	ILE	N-CA-C	-5.07	100.35	107.75
1	A	92	ALA	O-C-N	5.07	127.93	122.15
1	A	466	GLY	O-C-N	-5.07	115.91	122.34
1	A	143	THR	N-CA-CB	-5.05	103.68	111.46
1	A	330	SER	N-CA-C	5.05	117.17	111.11
1	A	323	ALA	N-CA-C	-5.05	102.39	109.96
1	B	278	ARG	NH1-CZ-NH2	-5.04	112.75	119.30
1	A	288	ALA	N-CA-C	-5.04	100.07	110.80
1	A	469	ILE	N-CA-C	5.01	115.62	110.36
1	A	308	THR	OG1-CB-CG2	5.01	119.33	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	GLU	CA-CB-CG	-5.01	104.08	114.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	HIS	Peptide
1	A	64	TYR	Sidechain
1	B	267	GLN	Mainchain
1	B	359	HIS	Peptide

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	3427	0	3501	131	0
1	B	3427	0	3501	84	0
2	A	53	0	31	2	0
2	B	53	0	30	1	0
3	A	212	0	0	14	0
3	B	239	0	0	4	0
All	All	7411	0	7063	205	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 15.

All (205) 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:468:ALA:CA	1:A:468:ALA:N	1.73	1.46
1:A:70:HIS:CD2	1:A:83:VAL:HG12	1.59	1.38
1:A:70:HIS:CD2	1:A:83:VAL:CG1	2.25	1.19
1:A:70:HIS:HD2	1:A:83:VAL:CG1	1.54	1.19
1:A:176:PHE:CE1	1:A:271:LYS:HE3	1.83	1.13
1:A:176:PHE:CD1	1:A:271:LYS:HE3	2.00	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:PHE:CE1	1:A:271:LYS:CE	2.56	0.88
1:B:465:SER:HB2	1:B:467:HIS:CE1	2.09	0.87
1:A:176:PHE:CZ	1:A:271:LYS:HG2	2.12	0.84
1:A:339:ARG:HA	1:A:343:HIS:HA	1.61	0.80
1:A:469:ILE:HB	1:A:470:HIS:ND1	1.98	0.78
1:A:71:GLU:O	1:A:71:GLU:HG2	1.83	0.77
1:B:290:SER:O	1:B:292:VAL:HG23	1.84	0.77
1:A:70:HIS:CD2	1:A:83:VAL:HG11	2.18	0.76
1:B:168:VAL:HG22	1:B:172:GLY:HA3	1.65	0.76
1:A:71:GLU:O	1:A:71:GLU:CG	2.33	0.74
1:A:81:GLY:HA2	3:A:627:HOH:O	1.86	0.74
1:A:146:VAL:HB	1:A:313:VAL:HG22	1.72	0.71
1:A:69:ALA:HB3	1:A:83:VAL:HG21	1.72	0.71
1:A:68:GLU:O	1:A:72:SER:HB2	1.90	0.71
1:A:438:THR:HG22	1:A:439:SER:O	1.91	0.69
1:B:36:LYS:HA	1:B:42:THR:HA	1.74	0.69
1:A:469:ILE:HD12	1:B:20:ILE:HD11	1.76	0.68
1:B:132:THR:HA	1:B:137:SER:O	1.93	0.68
1:B:254:VAL:O	1:B:268:ALA:HA	1.95	0.67
1:A:254:VAL:O	1:A:268:ALA:HA	1.96	0.65
1:A:82:GLU:HG3	3:A:649:HOH:O	1.97	0.65
1:B:271:LYS:HE2	3:B:612:HOH:O	1.98	0.64
1:B:124:LEU:HD23	1:B:128:LYS:HB2	1.80	0.64
1:A:471:VAL:CG2	1:A:472:ALA:N	2.61	0.63
1:A:183:LEU:HB3	1:A:206:VAL:HG12	1.82	0.62
1:A:471:VAL:HG23	1:A:472:ALA:CB	2.30	0.62
1:A:82:GLU:OE1	1:A:82:GLU:HA	1.98	0.62
1:B:407:ASP:O	1:B:411:ASP:HA	1.99	0.62
1:A:317:GLY:O	1:A:320:VAL:HG12	1.99	0.61
1:A:166:VAL:CG1	1:A:254:VAL:HG22	2.31	0.61
1:A:176:PHE:CZ	1:A:271:LYS:CG	2.85	0.60
1:A:82:GLU:CG	3:A:649:HOH:O	2.50	0.60
1:B:442:ASP:O	1:B:446:MET:HG3	2.02	0.60
1:A:80:THR:OG1	1:A:81:GLY:N	2.35	0.59
1:A:371:ALA:O	1:A:375:GLU:HG2	2.02	0.59
1:B:160:ALA:HB1	1:B:167:ILE:HD11	1.83	0.59
1:A:438:THR:HG23	1:A:442:ASP:HB2	1.85	0.59
1:A:22:SER:HB3	1:A:27:LEU:HD12	1.86	0.58
1:A:226:GLU:HG3	1:A:230:ILE:HD12	1.84	0.58
1:A:471:VAL:HG22	1:A:472:ALA:N	2.19	0.58
1:B:252:LYS:H	1:B:252:LYS:HE2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ARG:N	3:A:563:HOH:O	2.30	0.58
1:B:194:GLU:O	1:B:198:VAL:HG23	2.04	0.57
1:A:159:PRO:O	1:A:247:THR:HB	2.03	0.57
1:A:130:GLU:HA	1:A:139:GLN:O	2.05	0.56
1:A:470:HIS:HA	1:B:108:LEU:HD21	1.87	0.56
1:B:249:VAL:HB	1:B:254:VAL:HG13	1.86	0.56
1:A:53:CYS:O	1:A:57:LYS:HD2	2.05	0.56
1:B:226:GLU:O	1:B:230:ILE:HG13	2.05	0.56
1:B:176:PHE:CZ	1:B:271:LYS:HG2	2.39	0.56
1:A:21:LYS:O	1:A:25:LEU:HG	2.06	0.56
1:A:411:ASP:O	1:A:439:SER:HA	2.05	0.56
1:A:402:VAL:HG11	1:A:457:LEU:HA	1.87	0.56
1:A:186:ILE:HD11	1:A:272:LEU:HD21	1.88	0.55
1:A:469:ILE:HB	1:A:470:HIS:CE1	2.42	0.55
1:A:21:LYS:HD3	1:A:334:VAL:HG13	1.89	0.55
1:A:122:LYS:HD3	1:A:287:ALA:H	1.71	0.55
1:A:166:VAL:HG13	1:A:254:VAL:HG22	1.88	0.55
1:A:432:ILE:HG12	1:B:446:MET:HE1	1.87	0.54
1:A:151:GLY:H	1:A:319:VAL:HG13	1.71	0.54
1:A:124:LEU:HA	1:A:287:ALA:HB2	1.90	0.54
1:A:69:ALA:HB3	1:A:83:VAL:CG2	2.38	0.54
1:B:183:LEU:HD13	1:B:271:LYS:HB3	1.89	0.54
1:A:4:PHE:O	1:A:143:THR:HA	2.07	0.53
1:B:173:ALA:HA	1:B:176:PHE:CE1	2.43	0.53
1:A:165:ASP:HB2	3:A:529:HOH:O	2.08	0.53
1:B:247:THR:HG22	1:B:256:VAL:HG22	1.90	0.53
1:B:168:VAL:CG2	1:B:172:GLY:HA3	2.38	0.53
1:B:305:TYR:HD1	1:B:339:ARG:NH2	2.07	0.53
1:B:167:ILE:HD12	1:B:272:LEU:HD23	1.91	0.53
1:A:257:LYS:HA	1:A:265:LYS:HB2	1.92	0.52
1:A:447:VAL:HG22	1:B:331:GLU:HG2	1.92	0.52
1:B:287:ALA:O	1:B:289:ASP:N	2.43	0.51
1:A:83:VAL:CG1	1:A:83:VAL:O	2.58	0.51
1:A:469:ILE:CG2	1:A:470:HIS:CE1	2.93	0.51
1:A:152:SER:OG	1:A:278:ARG:HB3	2.10	0.51
1:A:331:GLU:HG3	1:B:447:VAL:HG22	1.91	0.51
1:A:471:VAL:HG23	1:A:472:ALA:HB3	1.92	0.51
1:B:356:ILE:HG12	1:B:362:ILE:HD12	1.92	0.51
1:A:213:ASP:HA	1:A:240:LEU:HB3	1.92	0.51
1:A:1:SER:HB3	3:A:678:HOH:O	2.10	0.50
1:B:367:LYS:O	1:B:417:HIS:HE1	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LYS:HB3	3:A:686:HOH:O	2.12	0.50
1:A:302:VAL:HB	1:A:306:CYS:HA	1.93	0.50
1:A:82:GLU:HG3	3:A:496:HOH:O	2.13	0.49
1:A:74:LYS:HD2	1:A:74:LYS:C	2.37	0.49
1:A:359:HIS:H	1:A:359:HIS:CD2	2.29	0.49
1:A:122:LYS:HD3	1:A:287:ALA:HA	1.95	0.49
1:A:446:MET:HE2	1:B:435:GLU:HG2	1.95	0.49
2:A:480:FAD:O1A	2:A:480:FAD:O4'	2.24	0.49
1:A:469:ILE:HB	1:A:470:HIS:HD1	1.75	0.49
1:A:351:LEU:HD21	1:A:434:MET:HE2	1.93	0.48
1:A:82:GLU:CD	3:A:649:HOH:O	2.55	0.48
1:B:375:GLU:O	1:B:377:VAL:HG23	2.13	0.48
1:A:390:GLY:CA	3:A:563:HOH:O	2.60	0.48
1:A:98:VAL:O	1:A:102:THR:HB	2.14	0.48
1:B:20:ILE:HD12	1:B:21:LYS:N	2.28	0.48
1:B:389:SER:HA	3:B:620:HOH:O	2.13	0.48
1:A:382:GLY:N	1:A:464:VAL:HG22	2.28	0.48
1:A:152:SER:HA	1:A:279:ARG:O	2.14	0.47
1:A:469:ILE:HD12	1:B:20:ILE:CD1	2.42	0.47
1:B:155:VAL:HG21	3:B:625:HOH:O	2.14	0.47
1:A:66:PHE:CE1	1:A:83:VAL:HG13	2.50	0.47
1:B:166:VAL:HG22	1:B:254:VAL:HG22	1.97	0.47
1:B:332:GLU:O	1:B:336:VAL:HG23	2.14	0.47
1:B:391:ARG:NH1	1:B:394:ALA:HB3	2.30	0.47
1:A:207:THR:HA	1:A:237:LYS:O	2.14	0.47
1:A:339:ARG:HA	1:A:343:HIS:CA	2.37	0.47
1:A:384:PHE:CE1	1:A:471:VAL:CG1	2.98	0.47
1:A:355:VAL:HG22	1:A:363:ALA:HB2	1.96	0.47
1:B:176:PHE:CZ	1:B:271:LYS:CG	2.98	0.47
1:B:206:VAL:O	1:B:237:LYS:HD3	2.15	0.47
1:A:9:ILE:HD11	1:A:129:VAL:HG11	1.98	0.46
1:B:150:SER:OG	1:B:319:VAL:HG11	2.14	0.46
1:A:35:TYR:O	1:A:42:THR:HA	2.14	0.46
1:A:222:GLN:HB2	1:A:403:LYS:HZ1	1.81	0.46
1:A:429:GLN:HG2	1:B:429:GLN:HG2	1.97	0.46
1:A:259:VAL:HA	1:A:263:GLY:HA2	1.98	0.46
1:A:372:LEU:O	1:A:377:VAL:HG13	2.15	0.46
1:A:468:ALA:N	1:A:468:ALA:C	2.65	0.46
1:B:74:LYS:HG3	1:B:75:LEU:HD22	1.96	0.46
1:B:250:LYS:O	1:B:252:LYS:HE2	2.16	0.46
1:A:258:PHE:HE1	1:A:266:SER:H	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:VAL:O	1:A:338:GLU:HG3	2.16	0.46
1:A:469:ILE:HG21	1:A:470:HIS:CE1	2.51	0.46
1:A:109:ILE:HB	1:A:114:VAL:HB	1.97	0.45
1:A:425:GLU:O	1:A:429:GLN:HG3	2.16	0.45
1:B:88:PRO:HG3	1:B:177:GLN:OE1	2.16	0.45
1:A:384:PHE:CE1	1:A:471:VAL:HG12	2.51	0.45
1:B:120:HIS:HE1	1:B:284:ASP:O	2.00	0.45
1:A:252:LYS:HG3	1:A:253:GLN:H	1.80	0.45
1:B:57:LYS:N	1:B:57:LYS:HE3	2.31	0.45
1:A:7:ILE:HG23	1:A:30:ALA:HB3	1.97	0.45
1:A:47:THR:O	1:A:52:GLY:N	2.50	0.45
1:B:183:LEU:CD1	1:B:271:LYS:HB3	2.47	0.45
1:A:1:SER:HA	3:A:545:HOH:O	2.17	0.45
1:A:450:HIS:ND1	1:A:451:PRO:HA	2.33	0.44
1:A:120:HIS:O	1:A:131:VAL:HA	2.16	0.44
1:A:432:ILE:HD12	1:B:429:GLN:HB3	1.99	0.44
1:B:302:VAL:HB	1:B:306:CYS:HA	1.99	0.44
1:A:68:GLU:O	1:A:72:SER:CB	2.63	0.44
1:B:153:LYS:HG2	1:B:281:VAL:CG2	2.48	0.44
1:B:167:ILE:CD1	1:B:272:LEU:HD23	2.48	0.44
1:B:335:VAL:HG12	1:B:339:ARG:NH1	2.32	0.44
1:A:166:VAL:HG11	1:A:249:VAL:HG13	1.99	0.44
1:A:176:PHE:CD1	1:A:271:LYS:CE	2.85	0.44
1:B:149:ALA:O	2:B:480:FAD:H52A	2.18	0.44
1:B:251:ASN:HB2	1:B:252:LYS:NZ	2.31	0.44
1:B:7:ILE:HD13	1:B:141:LEU:HD12	1.99	0.43
1:B:108:LEU:O	1:B:112:ASN:HB2	2.19	0.43
1:B:354:ALA:O	1:B:363:ALA:HA	2.18	0.43
1:B:328:LYS:HE2	1:B:332:GLU:OE2	2.17	0.43
1:B:331:GLU:HA	1:B:334:VAL:HG22	2.00	0.43
1:B:9:ILE:HD12	1:B:148:LEU:HD23	1.99	0.43
1:B:123:LEU:HD11	1:B:313:VAL:HG11	2.00	0.43
1:A:70:HIS:HD2	1:A:83:VAL:HG11	1.55	0.43
1:B:95:ASP:HA	1:B:98:VAL:HG22	1.99	0.43
1:B:152:SER:HB3	1:B:318:ASP:HB3	2.01	0.43
1:A:3:LYS:HA	1:A:142:ASP:O	2.19	0.43
1:B:316:ILE:CG2	1:B:336:VAL:HG21	2.49	0.43
1:A:1:SER:HB2	1:A:140:VAL:O	2.19	0.43
1:A:88:PRO:O	1:A:91:ILE:HD13	2.18	0.43
1:B:166:VAL:HG11	1:B:249:VAL:HG21	2.00	0.42
1:A:13:PRO:HD3	1:A:45:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LEU:HD11	1:A:101:LEU:HB3	2.01	0.42
1:A:359:HIS:CD2	1:A:359:HIS:N	2.86	0.42
1:A:9:ILE:HG12	1:A:32:ILE:HD12	2.02	0.42
1:A:220:ASP:OD1	1:A:403:LYS:NZ	2.51	0.42
1:B:153:LYS:HG2	1:B:281:VAL:HG22	2.01	0.42
1:B:296:GLU:HB2	3:B:715:HOH:O	2.19	0.42
1:B:7:ILE:HG12	1:B:30:ALA:HB3	2.01	0.42
1:B:49:LEU:HD21	1:B:101:LEU:CB	2.48	0.42
1:A:67:HIS:CD2	1:A:201:ARG:HD2	2.55	0.42
1:A:301:TYR:O	1:A:308:THR:HG22	2.20	0.42
1:A:349:TYR:HB2	3:A:484:HOH:O	2.20	0.42
1:B:198:VAL:O	1:B:202:LEU:HG	2.20	0.42
1:A:222:GLN:HB2	1:A:403:LYS:NZ	2.34	0.42
1:A:429:GLN:HG2	1:B:429:GLN:CG	2.50	0.42
1:B:367:LYS:O	1:B:417:HIS:CE1	2.72	0.41
1:A:301:TYR:HD1	3:A:587:HOH:O	2.02	0.41
1:A:314:TYR:HE2	1:A:339:ARG:HH21	1.68	0.41
1:B:120:HIS:O	1:B:131:VAL:HA	2.21	0.41
1:B:133:ALA:HB3	1:B:137:SER:HB2	2.02	0.41
1:B:372:LEU:HD12	1:B:372:LEU:HA	1.85	0.41
1:A:122:LYS:HD3	1:A:287:ALA:N	2.34	0.41
1:B:393:MET:HE2	1:B:393:MET:HB3	1.91	0.41
1:A:42:THR:HG21	1:A:118:GLU:HG2	2.03	0.41
1:A:54:ILE:HD13	1:A:54:ILE:HA	1.88	0.41
1:A:108:LEU:HD11	1:B:470:HIS:C	2.46	0.41
1:A:125:ALA:HB2	1:A:289:ASP:O	2.21	0.41
1:A:383:VAL:HG22	1:A:403:LYS:HG3	2.02	0.41
2:A:480:FAD:H9	2:A:480:FAD:H1'1	1.81	0.41
1:B:54:ILE:HB	1:B:55:PRO:HD3	2.02	0.41
1:A:93:ARG:NH1	1:B:396:ASN:HB2	2.36	0.40
1:B:453:LEU:HA	1:B:453:LEU:HD23	1.87	0.40
1:A:369:GLU:N	3:A:676:HOH:O	2.54	0.40
1:B:49:LEU:HD21	1:B:101:LEU:HB3	2.04	0.40
1:B:109:ILE:HB	1:B:114:VAL:HB	2.04	0.40
1:A:6:VAL:HG23	1:A:27:LEU:HD13	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	470/476 (99%)	419 (89%)	37 (8%)	14 (3%)	3	1
1	B	470/476 (99%)	425 (90%)	32 (7%)	13 (3%)	4	2
All	All	940/952 (99%)	844 (90%)	69 (7%)	27 (3%)	3	2

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	3	LYS
1	A	190	VAL
1	B	251	ASN
1	B	289	ASP
1	B	291	GLY
1	B	343	HIS
1	B	344	LYS
1	B	376	GLY
1	B	411	ASP
1	B	471	VAL
1	A	39	GLU
1	A	127	LYS
1	A	251	ASN
1	A	268	ALA
1	A	287	ALA
1	B	134	ALA
1	B	268	ALA
1	A	72	SER
1	A	283	THR
1	A	342	GLY
1	A	82	GLU
1	A	83	VAL
1	A	343	HIS
1	B	321	ARG

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Mol	Chain	Res	Type
1	B	288	ALA
1	B	454	SER

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	352/359 (98%)	276 (78%)	76 (22%)	1	1
1	B	352/359 (98%)	294 (84%)	58 (16%)	2	2
All	All	704/718 (98%)	570 (81%)	134 (19%)	1	1

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	34	LYS
1	A	38	LYS
1	A	51	VAL
1	A	55	PRO
1	A	56	SER
1	A	57	LYS
1	A	71	GLU
1	A	72	SER
1	A	74	LYS
1	A	80	THR
1	A	82	GLU
1	A	83	VAL
1	A	85	ILE
1	A	91	ILE
1	A	99	ARG
1	A	101	LEU
1	A	102	THR
1	A	108	LEU
1	A	109	ILE
1	A	110	LYS

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Mol	Chain	Res	Type
1	A	116	LEU
1	A	135	ASP
1	A	138	SER
1	A	139	GLN
1	A	141	LEU
1	A	164	GLN
1	A	168	VAL
1	A	175	ASP
1	A	178	ASN
1	A	190	VAL
1	A	195	LEU
1	A	202	LEU
1	A	209	LEU
1	A	213	ASP
1	A	214	LYS
1	A	222	GLN
1	A	231	LEU
1	A	232	THR
1	A	238	ILE
1	A	244	VAL
1	A	247	THR
1	A	252	LYS
1	A	254	VAL
1	A	256	VAL
1	A	257	LYS
1	A	265	LYS
1	A	266	SER
1	A	267	GLN
1	A	271	LYS
1	A	282	THR
1	A	289	ASP
1	A	293	THR
1	A	294	LEU
1	A	295	ASP
1	A	301	TYR
1	A	309	SER
1	A	311	PRO
1	A	320	VAL
1	A	321	ARG
1	A	335	VAL
1	A	358	THR
1	A	359	HIS

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Mol	Chain	Res	Type
1	A	368	THR
1	A	377	VAL
1	A	389	SER
1	A	393	MET
1	A	396	ASN
1	A	409	LYS
1	A	418	VAL
1	A	419	ILE
1	A	426	LEU
1	A	441	GLU
1	A	465	SER
1	A	469	ILE
1	A	471	VAL
1	B	2	GLN
1	B	3	LYS
1	B	21	LYS
1	B	28	LYS
1	B	32	ILE
1	B	49	LEU
1	B	51	VAL
1	B	55	PRO
1	B	57	LYS
1	B	70	HIS
1	B	74	LYS
1	B	83	VAL
1	B	85	ILE
1	B	90	MET
1	B	99	ARG
1	B	107	SER
1	B	109	ILE
1	B	123	LEU
1	B	124	LEU
1	B	162	VAL
1	B	168	VAL
1	B	170	SER
1	B	178	ASN
1	B	209	LEU
1	B	221	GLU
1	B	229	LYS
1	B	236	LEU
1	B	239	LEU
1	B	243	ARG

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Mol	Chain	Res	Type
1	B	244	VAL
1	B	249	VAL
1	B	250	LYS
1	B	252	LYS
1	B	254	VAL
1	B	255	THR
1	B	257	LYS
1	B	264	GLU
1	B	266	SER
1	B	271	LYS
1	B	279	ARG
1	B	290	SER
1	B	293	THR
1	B	294	LEU
1	B	309	SER
1	B	320	VAL
1	B	327	HIS
1	B	331	GLU
1	B	356	ILE
1	B	358	THR
1	B	372	LEU
1	B	373	LYS
1	B	418	VAL
1	B	427	VAL
1	B	441	GLU
1	B	443	LEU
1	B	465	SER
1	B	467	HIS
1	B	471	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	67	HIS
1	A	70	HIS
1	A	100	ASN
1	A	112	ASN
1	A	120	HIS
1	A	139	GLN
1	A	145	ASN
1	A	164	GLN

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Mol	Chain	Res	Type
1	A	222	GLN
1	A	359	HIS
1	A	380	ASN
1	A	458	HIS
1	B	24	GLN
1	B	67	HIS
1	B	120	HIS
1	B	139	GLN
1	B	164	GLN
1	B	228	GLN
1	B	234	GLN
1	B	251	ASN
1	B	417	HIS
1	B	458	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	480	-	58,58,58	2.35	10 (17%)	85,89,89	2.06	22 (25%)
2	FAD	A	480	-	58,58,58	1.36	5 (8%)	85,89,89	1.89	16 (18%)

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	480	-	-	3/34/50/50	0/6/6/6
2	FAD	A	480	-	-	2/34/50/50	0/6/6/6

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	480	FAD	C1'-C2'	-15.02	1.31	1.52
2	A	480	FAD	P-O5'	-4.67	1.41	1.59
2	A	480	FAD	C5A-N7A	-3.63	1.32	1.39
2	A	480	FAD	C1'-N10	-3.54	1.39	1.47
2	B	480	FAD	O2-C2	-3.24	1.18	1.24
2	B	480	FAD	PA-O3P	-2.95	1.56	1.59
2	B	480	FAD	C5A-N7A	-2.94	1.33	1.39
2	A	480	FAD	C4X-N5	2.67	1.36	1.30
2	B	480	FAD	C1'-N10	2.55	1.54	1.47
2	B	480	FAD	C6-C7	-2.33	1.36	1.39
2	A	480	FAD	C5X-N5	-2.27	1.35	1.39
2	B	480	FAD	C5X-N5	-2.08	1.35	1.39
2	B	480	FAD	C5'-C4'	2.07	1.54	1.51
2	B	480	FAD	C4A-N9A	-2.03	1.33	1.37
2	B	480	FAD	PA-O2A	-2.03	1.46	1.55

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	480	FAD	C5A-C4A-N3A	-7.60	116.25	126.72
2	B	480	FAD	N3A-C4A-N9A	6.49	138.21	127.17
2	A	480	FAD	N3A-C4A-N9A	6.37	138.01	127.17
2	B	480	FAD	C5A-C4A-N3A	-5.82	118.70	126.72
2	A	480	FAD	C6A-C5A-C4A	5.07	124.10	117.18
2	B	480	FAD	C6A-C5A-N7A	-4.68	123.06	132.09
2	B	480	FAD	C6A-C5A-C4A	4.47	123.29	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	480	FAD	O2'-C2'-C1'	4.30	127.87	110.20
2	A	480	FAD	C6A-C5A-N7A	-4.23	123.94	132.09
2	B	480	FAD	O4B-C1B-N9A	4.12	116.00	108.09
2	A	480	FAD	N3A-C2A-N1A	-3.97	122.56	128.58
2	B	480	FAD	C4-N3-C2	-3.84	118.81	125.64
2	B	480	FAD	C4A-N9A-C8A	3.81	109.74	105.74
2	B	480	FAD	C4X-C10-N10	3.79	121.91	116.48
2	A	480	FAD	C2A-N3A-C4A	3.43	120.20	111.83
2	B	480	FAD	O2-C2-N1	-3.14	116.59	121.80
2	A	480	FAD	C4-N3-C2	-3.10	120.14	125.64
2	B	480	FAD	C10-C4X-N5	-3.05	118.59	124.81
2	B	480	FAD	C1'-N10-C9A	2.87	126.20	120.63
2	B	480	FAD	N3A-C2A-N1A	-2.86	124.25	128.58
2	A	480	FAD	C4X-C10-N10	2.81	120.51	116.48
2	B	480	FAD	N6A-C6A-N1A	2.78	124.57	118.38
2	B	480	FAD	C4A-C5A-N7A	2.68	113.65	110.58
2	B	480	FAD	N9A-C8A-N7A	-2.65	110.18	113.94
2	A	480	FAD	C2'-C1'-N10	2.62	122.57	110.20
2	B	480	FAD	C5A-C4A-N9A	-2.49	103.09	105.81
2	B	480	FAD	C4-C4X-N5	2.44	121.58	118.21
2	A	480	FAD	C4-C4X-N5	2.41	121.53	118.21
2	A	480	FAD	C10-N1-C2	2.36	121.96	116.85
2	A	480	FAD	O4-C4-C4X	-2.33	120.38	126.53
2	A	480	FAD	O5'-P-O1P	-2.27	99.92	108.94
2	B	480	FAD	C2A-N3A-C4A	2.27	117.38	111.83
2	A	480	FAD	O2P-P-O5'	2.24	117.70	107.57
2	A	480	FAD	C10-C4X-N5	-2.19	120.34	124.81
2	A	480	FAD	O2'-C2'-C3'	2.16	114.30	109.25
2	B	480	FAD	C2B-C1B-N9A	-2.15	107.96	113.30
2	B	480	FAD	O4-C4-C4X	-2.08	121.03	126.53
2	B	480	FAD	C9A-N10-C10	-2.08	117.58	120.75

There are no chirality outliers.

All (5) torsion outliers are listed below:

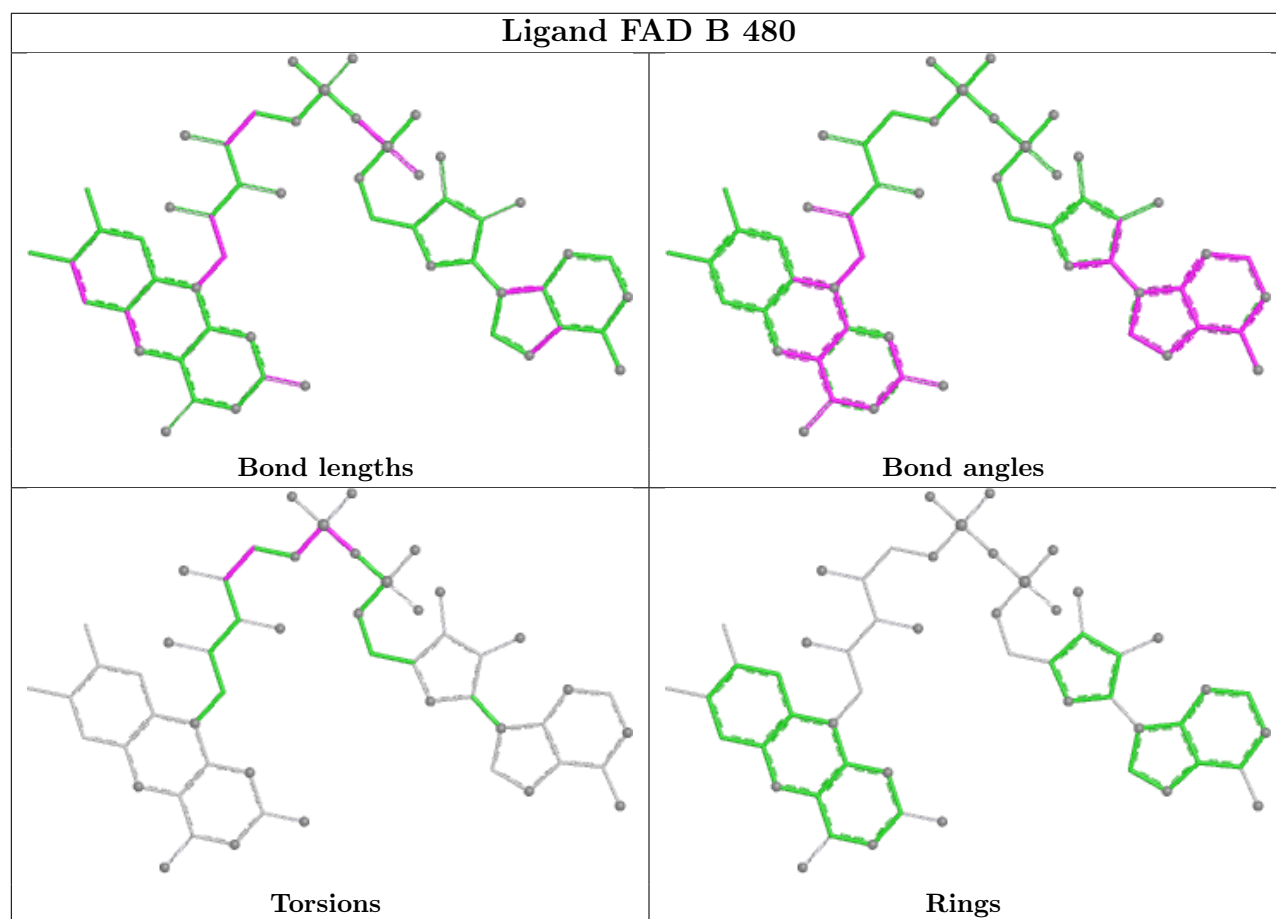
Mol	Chain	Res	Type	Atoms
2	B	480	FAD	C5'-O5'-P-O2P
2	B	480	FAD	PA-O3P-P-O5'
2	A	480	FAD	PA-O3P-P-O5'
2	A	480	FAD	O4B-C4B-C5B-O5B
2	B	480	FAD	O4'-C4'-C5'-O5'

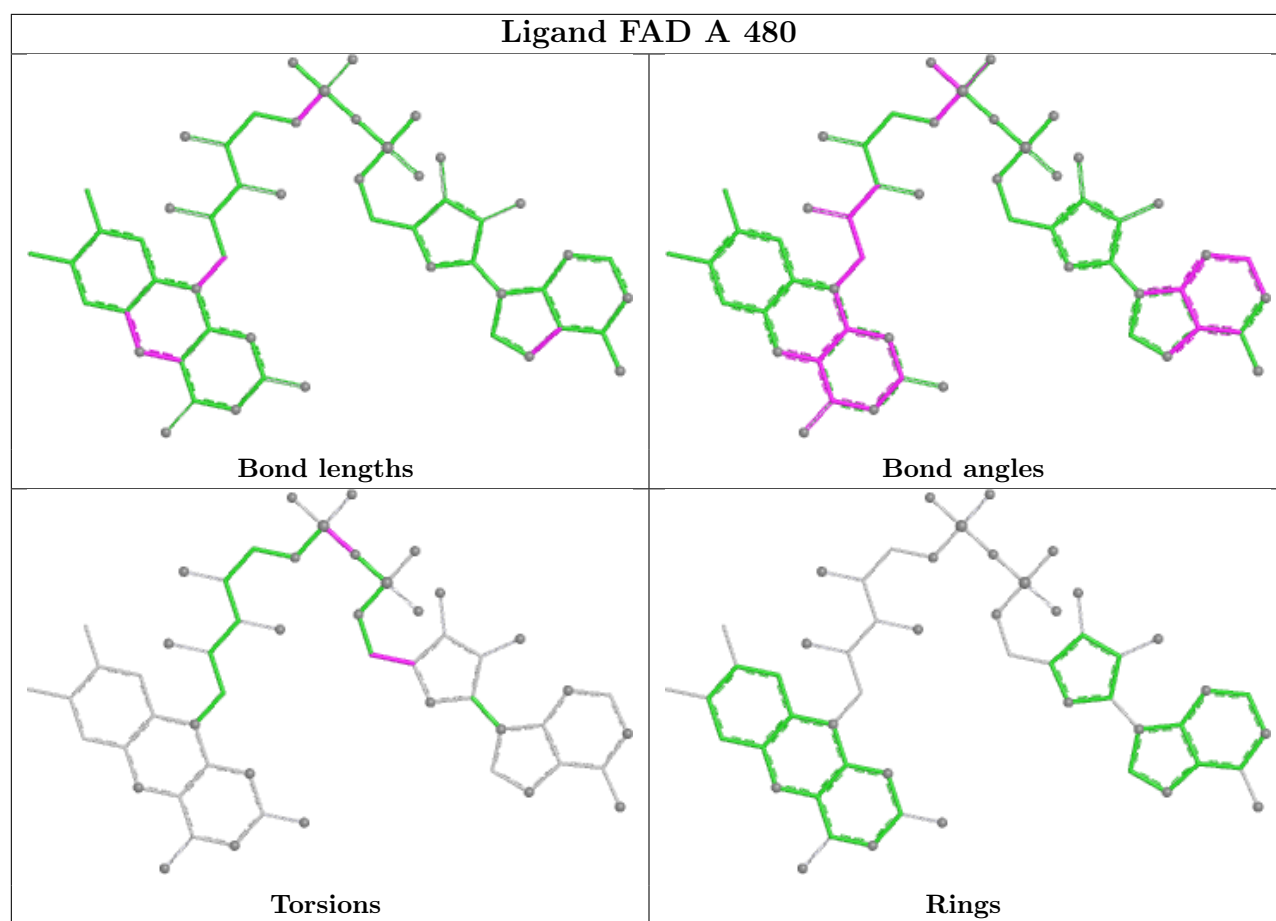
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	480	FAD	1	0
2	A	480	FAD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.