



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:11 AM UTC

PDB ID : 1LPF / pdb_00001lpf
Title : THREE-DIMENSIONAL STRUCTURE OF LIPOAMIDE DEHYDROGENASE FROM PSEUDOMONAS FLUORESCENS AT 2.8 ANGSTROMS RESOLUTION. ANALYSIS OF REDOX AND THERMOSTABILITY PROPERTIES
Authors : Mattevi, A.; Hol, W.
Deposited on : 1992-10-26
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) 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	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

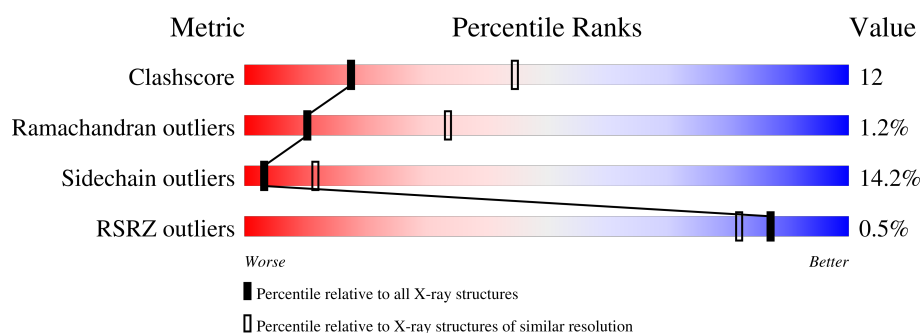
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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 $\leq 5\%$. 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	477	
1	B	477	

2 Entry composition (i)

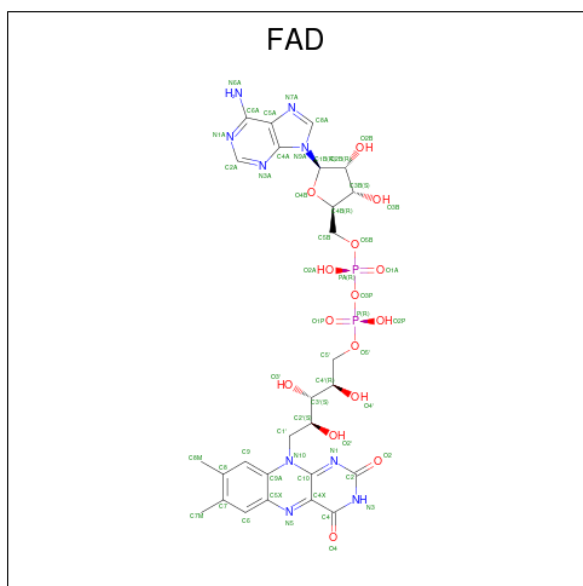
There are 2 unique types of molecules in this entry. The entry contains 6962 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3428	C 2172	N 588	O 656	S 12	0	0	0
1	B	472	Total 3428	C 2172	N 588	O 656	S 12	0	0	0

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

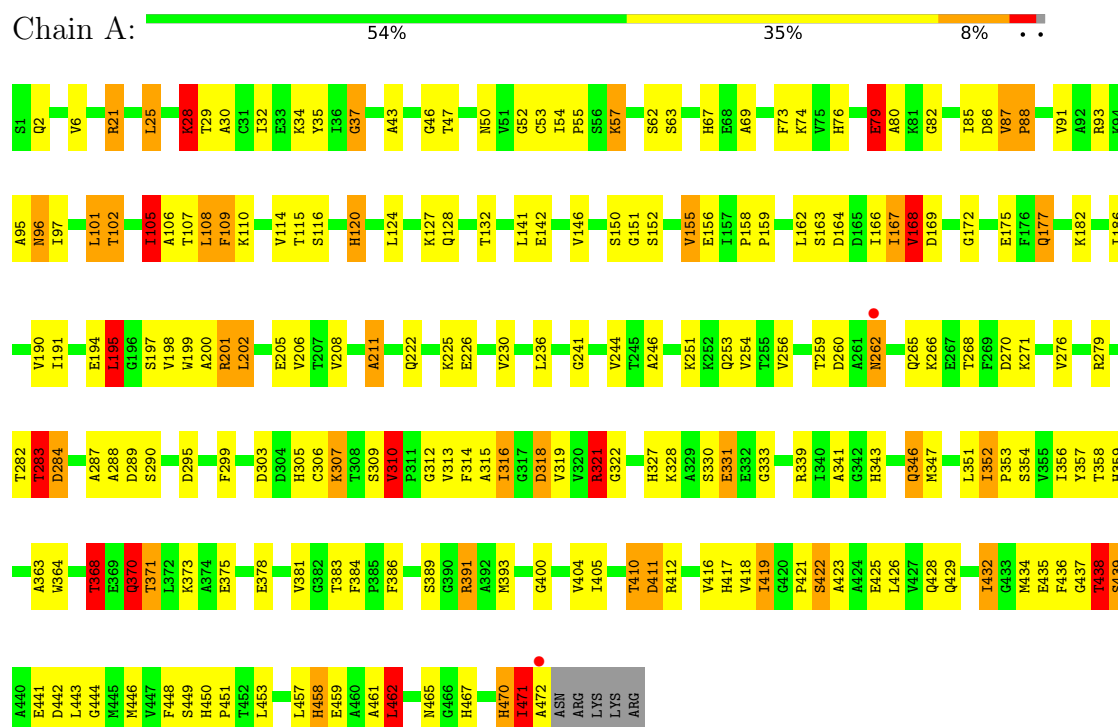


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

3 Residue-property plots

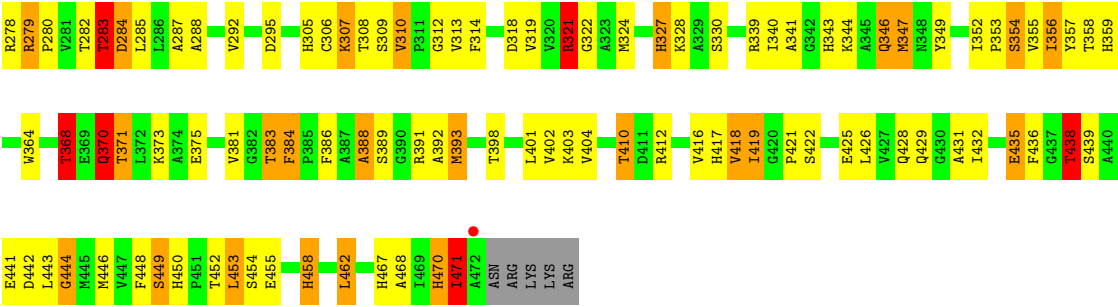
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	113.60Å 66.40Å 164.30Å 90.00° 99.20° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80 10.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.80) 76.9 (10.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.22 (at 2.81Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.192 , (Not available) 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6962	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 6.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.43	28/3480 (0.8%)	2.08	133/4725 (2.8%)
1	B	1.39	34/3480 (1.0%)	2.06	125/4725 (2.6%)
All	All	1.41	62/6960 (0.9%)	2.07	258/9450 (2.7%)

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	ILE	CA-CB	8.48	1.65	1.54
1	B	155	VAL	CA-CB	-7.90	1.45	1.54
1	B	458	HIS	CA-CB	-7.60	1.41	1.53
1	B	458	HIS	CG-ND1	-7.22	1.30	1.38
1	B	167	ILE	CA-CB	-7.04	1.46	1.54
1	A	462	LEU	CA-CB	-7.03	1.42	1.53
1	B	453	LEU	CA-CB	-6.95	1.42	1.53
1	B	76	HIS	CD2-NE2	-6.61	1.30	1.37
1	A	305	HIS	CD2-NE2	-6.57	1.30	1.37
1	B	305	HIS	CD2-NE2	-6.53	1.30	1.37
1	A	205	GLU	CA-CB	-6.51	1.44	1.52
1	B	359	HIS	CD2-NE2	-6.43	1.30	1.37
1	B	470	HIS	CD2-NE2	-6.39	1.30	1.37
1	A	467	HIS	CG-ND1	-6.29	1.31	1.38
1	B	87	VAL	CA-CB	-6.28	1.50	1.54
1	B	67	HIS	CD2-NE2	-6.25	1.30	1.37
1	B	343	HIS	CG-ND1	-6.23	1.31	1.38
1	B	343	HIS	CD2-NE2	-6.12	1.31	1.37
1	A	120	HIS	CG-ND1	-6.11	1.31	1.38
1	B	458	HIS	CD2-NE2	-6.05	1.31	1.37
1	A	471	ILE	CA-CB	5.98	1.62	1.54
1	B	467	HIS	CG-ND1	-5.97	1.31	1.38
1	B	327	HIS	CD2-NE2	-5.96	1.31	1.37
1	A	459	GLU	CA-CB	-5.95	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	HIS	CG-ND1	-5.94	1.31	1.38
1	B	467	HIS	CD2-NE2	-5.92	1.31	1.37
1	A	467	HIS	CD2-NE2	-5.91	1.31	1.37
1	B	92	ALA	CA-CB	-5.84	1.44	1.53
1	A	331	GLU	CA-C	-5.81	1.45	1.52
1	A	167	ILE	CA-CB	-5.81	1.46	1.53
1	B	190	VAL	CA-CB	-5.77	1.46	1.54
1	A	458	HIS	CD2-NE2	-5.76	1.31	1.37
1	A	432	ILE	CA-CB	-5.62	1.47	1.54
1	A	343	HIS	CD2-NE2	-5.62	1.31	1.37
1	A	404	VAL	CA-CB	-5.62	1.47	1.54
1	A	417	HIS	CD2-NE2	-5.59	1.31	1.37
1	A	359	HIS	CD2-NE2	-5.58	1.31	1.37
1	A	343	HIS	CG-ND1	-5.58	1.32	1.38
1	B	450	HIS	CD2-NE2	-5.49	1.31	1.37
1	B	305	HIS	CG-ND1	-5.49	1.32	1.38
1	A	67	HIS	CD2-NE2	-5.46	1.31	1.37
1	B	115	THR	CA-CB	5.45	1.60	1.53
1	A	470	HIS	CD2-NE2	-5.42	1.31	1.37
1	A	417	HIS	CG-ND1	-5.42	1.32	1.38
1	B	76	HIS	CG-ND1	-5.41	1.32	1.38
1	B	161	PRO	CA-CB	-5.37	1.47	1.53
1	B	105	ILE	CA-CB	5.37	1.61	1.54
1	B	450	HIS	CG-ND1	-5.37	1.32	1.38
1	A	450	HIS	CD2-NE2	-5.33	1.31	1.37
1	B	11	ALA	CA-C	5.32	1.59	1.53
1	A	76	HIS	CG-ND1	-5.32	1.32	1.38
1	B	417	HIS	CD2-NE2	-5.29	1.32	1.37
1	B	120	HIS	CG-ND1	-5.15	1.32	1.38
1	B	223	ILE	CA-CB	-5.11	1.47	1.54
1	B	418	VAL	CA-CB	5.09	1.62	1.54
1	A	327	HIS	CG-ND1	-5.08	1.32	1.38
1	B	308	THR	CA-CB	5.08	1.60	1.53
1	B	257	THR	CA-CB	5.07	1.61	1.53
1	A	200	ALA	CA-CB	-5.06	1.45	1.53
1	A	253	GLN	CA-CB	-5.06	1.45	1.53
1	A	450	HIS	CG-ND1	-5.04	1.32	1.38
1	A	405	ILE	CA-CB	-5.02	1.48	1.54

All (258) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	VAL	N-CA-CB	-13.51	97.31	112.45
1	A	168	VAL	N-CA-CB	-12.31	96.72	112.60
1	A	260	ASP	CA-CB-CG	9.94	122.54	112.60
1	A	371	THR	N-CA-C	-9.89	100.49	111.07
1	A	54	ILE	N-CA-CB	-9.88	104.28	110.50
1	B	164	ASP	CA-CB-CG	9.84	122.44	112.60
1	B	260	ASP	CA-CB-CG	9.81	122.42	112.60
1	A	467	HIS	N-CA-C	9.79	124.28	110.68
1	A	458	HIS	ND1-CG-CD2	9.46	115.56	106.10
1	B	228	LEU	O-C-N	9.30	131.98	122.12
1	B	384	PHE	CA-CB-CG	-9.29	104.51	113.80
1	B	458	HIS	ND1-CG-CD2	9.19	115.29	106.10
1	A	305	HIS	ND1-CG-CD2	9.18	115.28	106.10
1	B	467	HIS	ND1-CG-CD2	8.87	114.97	106.10
1	B	67	HIS	ND1-CG-CD2	8.87	114.97	106.10
1	B	368	THR	N-CA-CB	-8.86	97.77	110.44
1	A	164	ASP	CA-CB-CG	8.52	121.12	112.60
1	A	96	ASN	CA-CB-CG	-8.33	104.27	112.60
1	A	467	HIS	ND1-CG-CD2	8.32	114.42	106.10
1	B	410	THR	N-CA-C	-8.22	98.67	110.59
1	B	96	ASN	CA-CB-CG	-8.17	104.43	112.60
1	A	169	ASP	CA-CB-CG	8.15	120.75	112.60
1	B	371	THR	N-CA-C	-8.07	102.18	110.97
1	B	343	HIS	ND1-CG-CD2	8.04	114.14	106.10
1	A	437	GLY	CA-C-O	-7.96	110.36	118.96
1	A	86	ASP	CA-CB-CG	7.93	120.53	112.60
1	A	458	HIS	CG-CD2-NE2	-7.71	99.49	107.20
1	B	467	HIS	N-CA-C	7.70	127.21	110.80
1	A	352	ILE	N-CA-C	-7.59	102.10	108.63
1	B	76	HIS	ND1-CG-CD2	7.54	113.64	106.10
1	A	384	PHE	CA-CB-CG	-7.52	106.28	113.80
1	A	268	THR	O-C-N	-7.42	113.77	123.13
1	A	359	HIS	ND1-CG-CD2	7.41	113.51	106.10
1	B	327	HIS	ND1-CG-CD2	7.36	113.46	106.10
1	B	305	HIS	ND1-CG-CD2	7.34	113.44	106.10
1	B	283	THR	CA-CB-OG1	-7.30	98.65	109.60
1	B	185	VAL	N-CA-C	-7.24	97.74	108.45
1	A	470	HIS	ND1-CG-CD2	7.23	113.33	106.10
1	B	435	GLU	N-CA-C	-7.22	103.42	111.28
1	B	169	ASP	CA-CB-CG	7.19	119.79	112.60
1	B	206	VAL	N-CA-C	7.16	118.61	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	120	HIS	ND1-CG-CD2	7.14	113.24	106.10
1	A	97	ILE	N-CA-C	-7.11	103.60	110.42
1	B	141	LEU	N-CA-C	-7.11	98.65	109.95
1	B	36	ILE	N-CA-C	-7.09	98.05	108.54
1	B	364	TRP	CG-CD2-CE3	7.09	140.99	133.90
1	A	305	HIS	CG-CD2-NE2	-7.07	100.13	107.20
1	A	327	HIS	ND1-CG-CD2	7.07	113.17	106.10
1	B	417	HIS	ND1-CG-CD2	7.06	113.16	106.10
1	A	450	HIS	ND1-CG-CD2	7.00	113.10	106.10
1	A	87	VAL	CB-CA-C	-6.98	107.07	113.70
1	A	175	GLU	N-CA-CB	-6.97	100.91	110.95
1	B	467	HIS	CG-CD2-NE2	-6.96	100.24	107.20
1	A	120	HIS	ND1-CG-CD2	6.94	113.04	106.10
1	A	343	HIS	ND1-CG-CD2	6.91	113.01	106.10
1	B	370	GLN	OE1-CD-NE2	-6.90	115.70	122.60
1	B	102	THR	N-CA-CB	-6.75	98.25	109.72
1	B	195	LEU	CD1-CG-CD2	-6.74	95.96	110.80
1	A	142	GLU	N-CA-C	-6.71	98.26	109.07
1	A	356	ILE	O-C-N	-6.70	116.22	123.18
1	A	164	ASP	CB-CA-C	-6.68	107.84	115.79
1	A	386	PHE	CA-CB-CG	-6.67	107.13	113.80
1	A	102	THR	N-CA-CB	-6.67	98.91	109.78
1	A	368	THR	N-CA-CB	-6.64	99.84	110.46
1	A	295	ASP	CA-CB-CG	6.59	119.19	112.60
1	B	416	VAL	N-CA-C	-6.59	98.88	108.11
1	A	417	HIS	ND1-CG-CD2	6.59	112.69	106.10
1	B	127	LYS	CB-CG-CD	-6.58	96.16	111.30
1	B	386	PHE	CA-CB-CG	-6.57	107.23	113.80
1	A	225	LYS	CA-CB-CG	6.57	127.24	114.10
1	B	458	HIS	CG-CD2-NE2	-6.57	100.63	107.20
1	A	128	GLN	N-CA-C	-6.53	99.56	109.95
1	A	168	VAL	CB-CA-C	6.53	120.13	111.19
1	A	467	HIS	CA-C-N	-6.48	113.05	122.19
1	A	467	HIS	C-N-CA	-6.48	113.05	122.19
1	B	356	ILE	O-C-N	-6.47	116.27	123.26
1	A	416	VAL	N-CA-C	-6.46	98.81	108.12
1	A	166	ILE	N-CA-C	-6.46	105.53	111.67
1	B	105	ILE	CB-CG1-CD1	-6.43	100.29	113.80
1	A	318	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	290	SER	O-C-N	6.40	130.14	122.27
1	A	67	HIS	ND1-CG-CD2	6.39	112.49	106.10
1	B	340	ILE	O-C-N	-6.39	115.63	121.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ASN	N-CA-C	6.39	117.91	111.07
1	A	310	VAL	CA-C-O	6.39	123.72	119.38
1	B	417	HIS	CG-CD2-NE2	-6.39	100.81	107.20
1	A	410	THR	N-CA-C	-6.33	101.41	110.59
1	B	186	ILE	N-CA-C	-6.33	98.01	107.37
1	B	419	ILE	N-CA-C	-6.33	99.25	108.11
1	B	283	THR	N-CA-C	6.31	124.23	110.80
1	A	434	MET	CG-SD-CE	-6.30	87.04	100.90
1	A	449	SER	CB-CA-C	-6.29	99.67	109.61
1	A	177	GLN	N-CA-C	-6.22	105.96	112.93
1	B	283	THR	CA-CB-CG2	6.21	121.05	110.50
1	B	128	GLN	N-CA-C	-6.20	99.30	109.40
1	B	223	ILE	N-CA-C	-6.17	104.49	110.72
1	A	76	HIS	ND1-CG-CD2	6.17	112.27	106.10
1	A	422	SER	N-CA-C	6.16	120.38	112.86
1	A	167	ILE	N-CA-C	-6.15	98.27	107.37
1	A	462	LEU	N-CA-C	-6.15	104.27	110.97
1	B	168	VAL	CB-CA-C	6.14	119.93	111.34
1	B	353	PRO	CA-C-O	-6.13	114.23	122.08
1	A	461	ALA	CA-C-O	6.09	126.87	120.42
1	A	155	VAL	N-CA-C	-6.07	100.95	109.21
1	A	251	LYS	CA-CB-CG	6.07	126.23	114.10
1	B	284	ASP	N-CA-C	-6.07	97.88	110.80
1	B	393	MET	CA-CB-CG	-6.05	101.99	114.10
1	B	295	ASP	CA-CB-CG	6.05	118.65	112.60
1	B	279	ARG	CA-C-N	6.01	125.77	119.76
1	B	279	ARG	C-N-CA	6.01	125.77	119.76
1	A	299	PHE	CA-CB-CG	-6.00	107.80	113.80
1	A	449	SER	N-CA-C	5.99	118.73	110.35
1	A	457	LEU	N-CA-C	-5.96	104.70	111.14
1	B	153	ARG	CA-C-N	5.95	126.29	119.93
1	B	153	ARG	C-N-CA	5.95	126.29	119.93
1	A	467	HIS	CG-CD2-NE2	-5.91	101.30	107.20
1	A	208	VAL	N-CA-C	-5.89	99.15	107.75
1	A	67	HIS	CB-CG-CD2	-5.88	123.56	131.20
1	B	470	HIS	ND1-CG-CD2	5.86	111.96	106.10
1	A	439	SER	N-CA-C	-5.86	101.32	110.17
1	A	53	CYS	CA-C-N	-5.85	116.55	120.24
1	A	53	CYS	C-N-CA	-5.85	116.55	120.24
1	B	327	HIS	CG-CD2-NE2	-5.83	101.38	107.20
1	A	97	ILE	CB-CG1-CD1	-5.82	101.58	113.80
1	A	441	GLU	CA-C-O	-5.82	114.38	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	ALA	CA-C-O	5.82	126.53	119.78
1	B	76	HIS	CG-CD2-NE2	-5.80	101.40	107.20
1	B	2	GLN	OE1-CD-NE2	-5.79	116.81	122.60
1	B	422	SER	N-CA-C	5.79	119.92	112.86
1	A	95	ALA	O-C-N	5.79	128.03	122.07
1	A	411	ASP	N-CA-C	-5.76	104.41	112.25
1	A	438	THR	CB-CA-C	-5.74	98.99	110.42
1	A	359	HIS	CA-CB-CG	-5.73	108.07	113.80
1	A	127	LYS	CB-CG-CD	-5.73	98.12	111.30
1	A	2	GLN	OE1-CD-NE2	-5.72	116.88	122.60
1	B	438	THR	CB-CA-C	-5.72	100.58	109.61
1	A	368	THR	CB-CA-C	5.71	119.82	109.83
1	A	283	THR	CA-CB-OG1	-5.70	101.06	109.60
1	B	449	SER	CB-CA-C	-5.69	100.62	109.61
1	A	162	LEU	CA-C-O	5.67	127.37	120.62
1	A	303	ASP	CA-CB-CG	5.67	118.27	112.60
1	B	470	HIS	N-CA-C	5.66	118.97	112.97
1	A	276	VAL	CA-CB-CG2	-5.66	100.78	110.40
1	B	346	GLN	OE1-CD-NE2	-5.64	116.96	122.60
1	B	155	VAL	CA-CB-CG2	-5.63	100.83	110.40
1	A	370	GLN	OE1-CD-NE2	-5.63	116.97	122.60
1	B	177	GLN	OE1-CD-NE2	-5.63	116.97	122.60
1	B	68	GLU	N-CA-C	-5.62	105.06	111.07
1	A	141	LEU	N-CA-C	-5.60	101.15	110.17
1	A	199	TRP	CG-CD2-CE3	5.60	139.50	133.90
1	B	67	HIS	CG-CD2-NE2	-5.60	101.60	107.20
1	A	177	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	A	206	VAL	N-CA-C	5.59	117.04	108.71
1	A	359	HIS	CG-CD2-NE2	-5.59	101.61	107.20
1	A	283	THR	CA-CB-CG2	5.55	119.94	110.50
1	B	102	THR	CB-CA-C	5.55	120.06	110.84
1	B	354	SER	O-C-N	-5.55	116.01	123.23
1	B	306	CYS	N-CA-C	5.55	119.87	113.38
1	B	449	SER	N-CA-C	5.54	118.11	110.35
1	B	356	ILE	N-CA-C	-5.53	100.36	108.11
1	A	211	ALA	N-CA-C	5.53	119.12	112.38
1	B	410	THR	CA-C-N	-5.52	114.33	122.83
1	B	410	THR	C-N-CA	-5.52	114.33	122.83
1	A	198	VAL	N-CA-C	5.52	115.72	110.42
1	B	251	LYS	CA-CB-CG	5.52	125.14	114.10
1	B	470	HIS	CG-CD2-NE2	-5.51	101.69	107.20
1	A	470	HIS	CG-CD2-NE2	-5.51	101.69	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	THR	CA-C-O	-5.49	112.66	120.51
1	A	114	VAL	O-C-N	5.48	128.94	123.18
1	B	96	ASN	N-CA-C	5.48	117.25	111.28
1	B	441	GLU	CA-C-O	-5.48	114.74	120.55
1	A	246	ALA	N-CA-C	5.48	117.59	108.99
1	B	359	HIS	ND1-CG-CD2	5.48	111.58	106.10
1	A	346	GLN	N-CA-C	-5.47	100.85	109.50
1	B	364	TRP	CB-CG-CD1	-5.47	118.69	126.90
1	B	142	GLU	N-CA-C	-5.46	100.29	109.07
1	A	102	THR	CA-CB-OG1	-5.46	101.42	109.60
1	A	43	ALA	CA-C-O	5.45	126.13	120.30
1	A	186	ILE	N-CA-C	-5.42	98.66	107.28
1	B	283	THR	N-CA-CB	-5.42	101.33	110.49
1	B	343	HIS	CG-CD2-NE2	-5.42	101.78	107.20
1	A	321	ARG	CB-CG-CD	5.41	123.74	111.30
1	B	404	VAL	N-CA-C	-5.40	100.53	108.85
1	B	65	LYS	CA-CB-CG	-5.39	103.31	114.10
1	A	132	THR	N-CA-C	-5.39	100.31	108.67
1	B	327	HIS	CB-CG-CD2	-5.39	124.19	131.20
1	A	315	ALA	O-C-N	-5.38	116.24	123.23
1	B	321	ARG	CB-CG-CD	5.37	123.66	111.30
1	B	431	ALA	N-CA-C	-5.37	105.32	111.07
1	B	444	GLY	O-C-N	-5.34	117.06	122.19
1	B	56	SER	CA-C-O	-5.32	115.23	120.82
1	A	378	GLU	N-CA-C	-5.32	100.57	109.24
1	B	267	GLU	O-C-N	-5.31	117.11	123.27
1	B	346	GLN	N-CA-C	-5.27	101.52	109.85
1	B	265	GLN	N-CA-C	-5.25	101.31	109.24
1	B	270	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	284	ASP	N-CA-C	-5.25	99.62	110.80
1	B	312	GLY	N-CA-C	-5.25	108.08	115.32
1	B	321	ARG	O-C-N	5.24	129.31	122.87
1	A	450	HIS	CG-CD2-NE2	-5.23	101.97	107.20
1	B	308	THR	N-CA-C	-5.23	102.25	110.36
1	A	28	LYS	N-CA-C	-5.22	101.26	109.25
1	A	151	GLY	O-C-N	5.22	127.39	122.90
1	A	438	THR	N-CA-CB	5.22	119.31	110.49
1	B	355	VAL	N-CA-C	-5.22	100.73	108.45
1	B	283	THR	O-C-N	-5.21	115.65	122.59
1	A	177	GLN	CG-CD-NE2	5.21	124.21	116.40
1	A	288	ALA	N-CA-C	5.19	119.09	112.34
1	A	312	GLY	N-CA-C	-5.19	108.18	114.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	LYS	CA-CB-CG	5.18	124.47	114.10
1	B	425	GLU	CB-CG-CD	5.18	121.41	112.60
1	A	276	VAL	CA-CB-CG1	5.18	119.20	110.40
1	B	176	PHE	CA-CB-CG	5.18	118.98	113.80
1	B	368	THR	CB-CA-C	5.17	121.09	110.40
1	B	171	THR	N-CA-C	5.15	116.58	111.07
1	B	448	PHE	CA-CB-CG	5.15	118.95	113.80
1	B	305	HIS	CG-CD2-NE2	-5.14	102.06	107.20
1	A	259	THR	CA-C-N	-5.14	117.63	123.13
1	A	259	THR	C-N-CA	-5.14	117.63	123.13
1	A	128	GLN	CA-C-N	-5.13	116.42	123.14
1	A	128	GLN	C-N-CA	-5.13	116.42	123.14
1	A	150	SER	CA-C-N	-5.13	113.99	122.05
1	A	150	SER	C-N-CA	-5.13	113.99	122.05
1	A	465	ASN	O-C-N	-5.12	115.06	121.97
1	B	269	PHE	CA-CB-CG	-5.12	108.68	113.80
1	B	364	TRP	CA-CB-CG	5.12	123.32	113.60
1	A	356	ILE	N-CA-C	-5.11	100.21	107.77
1	A	364	TRP	CE2-CD2-CG	-5.11	101.07	107.20
1	A	405	ILE	N-CA-C	-5.11	100.96	108.11
1	B	280	PRO	CA-C-N	-5.10	116.37	122.90
1	B	280	PRO	C-N-CA	-5.10	116.37	122.90
1	A	315	ALA	CA-C-O	-5.10	115.19	120.70
1	A	364	TRP	CG-CD2-CE3	5.10	139.00	133.90
1	B	222	GLN	CG-CD-NE2	5.09	124.04	116.40
1	A	410	THR	CA-C-N	-5.09	114.50	122.95
1	A	410	THR	C-N-CA	-5.09	114.50	122.95
1	B	177	GLN	N-CA-CB	-5.08	103.10	110.47
1	B	127	LYS	CA-C-N	-5.08	115.33	122.94
1	B	127	LYS	C-N-CA	-5.08	115.33	122.94
1	B	208	VAL	N-CA-C	-5.07	100.34	107.75
1	B	388	ALA	CA-C-N	-5.06	116.04	122.77
1	B	388	ALA	C-N-CA	-5.06	116.04	122.77
1	A	470	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	A	448	PHE	CA-C-O	-5.05	114.83	120.54
1	B	58	ALA	O-C-N	-5.05	116.06	122.27
1	A	289	ASP	N-CA-CB	-5.05	104.22	111.54
1	A	195	LEU	CD1-CG-CD2	-5.05	99.70	110.80
1	A	343	HIS	CG-CD2-NE2	-5.04	102.16	107.20
1	A	417	HIS	O-C-N	-5.04	117.41	123.31
1	B	249	VAL	N-CA-C	-5.04	102.35	109.21
1	B	256	VAL	CA-CB-CG2	-5.04	101.84	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	429	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	B	57	LYS	CB-CA-C	-5.03	102.76	110.81
1	A	79	GLU	CB-CA-C	-5.02	103.29	111.68
1	B	132	THR	N-CA-C	-5.02	99.59	108.23
1	B	292	VAL	N-CA-CB	-5.01	105.06	110.53
1	B	167	ILE	N-CA-C	-5.01	100.67	107.99
1	A	417	HIS	CG-CD2-NE2	-5.01	102.19	107.20

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	3428	0	3470	96	0
1	B	3428	0	3470	93	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
All	All	6962	0	7002	173	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 12.

All (173) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ASN:H	1:B:262:ASN:HD22	1.12	0.97
1:B:262:ASN:HD22	1:B:262:ASN:N	1.63	0.94
1:A:262:ASN:HD22	1:A:262:ASN:N	1.65	0.93
1:A:262:ASN:H	1:A:262:ASN:ND2	1.69	0.87
1:A:262:ASN:HD22	1:A:262:ASN:H	0.88	0.85
1:B:262:ASN:H	1:B:262:ASN:ND2	1.83	0.76
1:B:146:VAL:HB	1:B:313:VAL:HG22	1.68	0.74
1:B:428:GLN:O	1:B:432:ILE:HG13	1.89	0.73
1:A:438:THR:HG23	1:B:436:PHE:CZ	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:VAL:HB	1:A:313:VAL:HG22	1.69	0.72
1:A:438:THR:HG23	1:B:436:PHE:HZ	1.54	0.71
1:A:436:PHE:CZ	1:B:438:THR:HG23	2.27	0.68
1:A:438:THR:HG21	1:A:443:LEU:HG	1.75	0.67
1:A:80:ALA:HB1	1:B:80:ALA:HB1	1.77	0.66
1:A:391:ARG:HG3	1:A:391:ARG:HH11	1.60	0.65
1:A:436:PHE:HZ	1:B:438:THR:HG23	1.62	0.65
1:B:158:PRO:HG2	1:B:159:PRO:HD3	1.79	0.64
1:A:158:PRO:HG2	1:A:159:PRO:HD3	1.81	0.62
1:A:52:GLY:O	1:A:55:PRO:HD2	1.99	0.62
1:B:370:GLN:NE2	1:B:370:GLN:H	1.97	0.62
1:A:88:PRO:HG3	1:A:177:GLN:HG3	1.80	0.62
1:B:35:TYR:HD2	1:B:43:ALA:HB3	1.65	0.62
1:A:310:VAL:HG22	1:A:313:VAL:HB	1.80	0.61
1:B:262:ASN:N	1:B:262:ASN:ND2	2.37	0.60
1:A:438:THR:HG22	1:A:442:ASP:HB2	1.83	0.60
1:A:351:LEU:O	1:A:353:PRO:HD3	2.02	0.59
1:B:347:MET:HG2	1:B:349:TYR:CE2	2.37	0.59
1:A:163:SER:H	1:A:167:ILE:HB	1.69	0.58
1:A:373:LYS:HA	1:A:373:LYS:HE2	1.87	0.56
1:B:307:LYS:HG2	1:B:314:PHE:HE1	1.71	0.56
1:B:87:VAL:HB	1:B:88:PRO:HD3	1.87	0.56
1:A:226:GLU:O	1:A:230:VAL:HG23	2.05	0.56
1:A:421:PRO:HB2	1:A:453:LEU:HD13	1.87	0.56
1:B:373:LYS:HE2	1:B:373:LYS:HA	1.87	0.56
1:A:87:VAL:O	1:A:91:VAL:HG23	2.05	0.56
1:A:322:GLY:HA3	1:A:328:LYS:HE3	1.88	0.56
1:B:310:VAL:HG22	1:B:313:VAL:HB	1.88	0.56
1:A:428:GLN:O	1:A:432:ILE:HG13	2.05	0.56
1:A:368:THR:HG22	1:A:371:THR:OG1	2.06	0.56
1:B:244:VAL:HG13	1:B:256:VAL:HG13	1.87	0.56
1:B:438:THR:HG22	1:B:442:ASP:HB2	1.88	0.55
1:B:438:THR:HG21	1:B:443:LEU:HG	1.88	0.55
1:A:244:VAL:HG13	1:A:256:VAL:HG13	1.88	0.55
1:B:444:GLY:O	1:B:458:HIS:HE1	1.89	0.54
1:B:51:VAL:CG1	1:B:171:THR:HG23	2.38	0.54
1:B:124:LEU:HD23	1:B:287:ALA:HB2	1.89	0.54
1:B:120:HIS:HE1	1:B:284:ASP:O	1.91	0.53
1:B:28:LYS:HZ1	1:B:29:THR:H	1.57	0.52
1:B:4:PHE:HD1	1:B:28:LYS:HG3	1.74	0.52
1:B:55:PRO:HB3	1:B:94:LYS:HD2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:MET:HG2	1:B:349:TYR:CZ	2.45	0.52
1:A:370:GLN:NE2	1:A:370:GLN:H	2.07	0.52
1:A:34:LYS:HZ2	1:A:120:HIS:HD2	1.57	0.51
1:A:101:LEU:HD11	1:B:393:MET:HE1	1.92	0.51
1:A:316:ILE:HD12	1:A:333:GLY:HA2	1.92	0.50
1:A:28:LYS:HZ2	1:A:28:LYS:HA	1.76	0.50
1:B:278:ARG:HB2	1:B:324:MET:HE1	1.94	0.50
1:A:435:GLU:HG2	1:B:446:MET:HE2	1.94	0.50
1:B:368:THR:HG22	1:B:371:THR:OG1	2.12	0.50
1:B:384:PHE:CZ	1:B:388:ALA:HB3	2.47	0.50
1:A:87:VAL:HB	1:A:88:PRO:HD3	1.92	0.50
1:B:163:SER:H	1:B:167:ILE:HB	1.77	0.49
1:B:191:ILE:O	1:B:195:LEU:HD23	2.12	0.49
1:A:106:ALA:O	1:A:109:PHE:HB2	2.12	0.49
1:A:34:LYS:NZ	1:A:120:HIS:HD2	2.10	0.49
1:B:35:TYR:CD2	1:B:43:ALA:HB3	2.46	0.49
1:B:148:ILE:HG21	1:B:285:LEU:HD21	1.92	0.49
1:B:391:ARG:HH11	1:B:391:ARG:HG3	1.78	0.48
1:A:411:ASP:O	1:A:439:SER:HA	2.14	0.48
1:B:105:ILE:HA	1:B:108:LEU:HB2	1.96	0.48
1:A:438:THR:CG2	1:B:436:PHE:HZ	2.26	0.48
1:A:110:LYS:HZ1	1:A:116:SER:HB2	1.79	0.48
1:A:120:HIS:HE1	1:A:284:ASP:O	1.97	0.48
1:B:156:GLU:HB2	1:B:279:ARG:HH22	1.79	0.48
1:A:339:ARG:HH21	1:A:346:GLN:NE2	2.12	0.48
1:A:30:ALA:HA	1:A:115:THR:O	2.15	0.47
1:A:93:ARG:HD3	1:B:75:VAL:O	2.14	0.47
1:B:322:GLY:HA3	1:B:328:LYS:HE3	1.96	0.47
1:A:25:LEU:HG	1:A:341:ALA:CB	2.45	0.47
1:B:226:GLU:O	1:B:230:VAL:HG23	2.15	0.47
1:B:32:ILE:HG22	2:B:480:FAD:H2A	1.96	0.47
1:B:60:LEU:HD13	1:B:357:TYR:O	2.14	0.47
1:A:28:LYS:HZ1	1:A:29:THR:H	1.61	0.47
1:A:57:LYS:HD3	1:A:57:LYS:HA	1.71	0.47
1:B:215:PHE:CE2	1:B:216:LEU:HD12	2.50	0.47
1:A:62:SER:HB3	1:B:76:HIS:HB3	1.97	0.46
1:A:74:LYS:HE3	1:A:79:GLU:OE2	2.13	0.46
1:B:421:PRO:HB2	1:B:453:LEU:HD13	1.97	0.46
1:A:211:ALA:O	1:A:241:GLY:HA2	2.16	0.46
1:A:307:LYS:HG2	1:A:314:PHE:HE1	1.81	0.46
1:B:371:THR:O	1:B:375:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:SER:O	1:A:423:ALA:C	2.59	0.45
1:A:262:ASN:N	1:A:262:ASN:ND2	2.39	0.45
1:A:425:GLU:HG3	1:B:454:SER:OG	2.16	0.45
1:B:191:ILE:HG22	1:B:195:LEU:HD23	1.98	0.45
1:A:57:LYS:HD2	1:A:357:TYR:CG	2.52	0.45
1:A:446:MET:HE2	1:B:435:GLU:HG2	1.98	0.45
1:B:462:LEU:HB3	1:B:468:ALA:HA	1.99	0.45
1:B:470:HIS:O	1:B:471:ILE:HG23	2.16	0.45
1:A:339:ARG:NH2	1:A:346:GLN:HE22	2.14	0.45
1:B:158:PRO:O	1:B:161:PRO:HG3	2.16	0.45
1:B:410:THR:HG21	1:B:412:ARG:NH2	2.32	0.45
1:A:432:ILE:CD1	1:B:429:GLN:HB3	2.47	0.45
1:B:6:VAL:HB	1:B:29:THR:HG23	1.98	0.45
1:B:53:CYS:O	1:B:57:LYS:HE2	2.16	0.45
1:A:470:HIS:O	1:A:471:ILE:HG23	2.17	0.45
1:B:120:HIS:CE1	1:B:284:ASP:O	2.69	0.45
1:A:354:SER:O	1:A:363:ALA:HA	2.16	0.45
1:B:16:TYR:O	1:B:20:ILE:HG13	2.17	0.45
1:A:190:VAL:O	1:A:194:GLU:HG3	2.16	0.44
1:A:444:GLY:O	1:A:458:HIS:HE1	2.00	0.44
1:B:49:LEU:HD21	1:B:101:LEU:HB3	1.99	0.44
1:B:57:LYS:HA	1:B:57:LYS:HD3	1.55	0.44
1:B:94:LYS:NZ	1:B:174:LEU:O	2.51	0.44
1:B:190:VAL:HG22	1:B:356:ILE:HG12	2.00	0.44
1:A:152:SER:HB3	1:A:318:ASP:HB3	2.00	0.44
1:A:462:LEU:HD12	1:A:462:LEU:HA	1.82	0.44
1:A:168:VAL:HG22	1:A:172:GLY:HA3	2.00	0.44
1:A:32:ILE:HG22	2:A:480:FAD:H2A	1.99	0.44
1:A:35:TYR:CE2	1:A:37:GLY:HA2	2.53	0.43
1:B:110:LYS:HA	1:B:110:LYS:HD3	1.88	0.43
1:B:215:PHE:HE1	1:B:238:ILE:HD13	1.83	0.43
1:A:202:LEU:HD23	1:A:202:LEU:N	2.33	0.43
1:A:451:PRO:HD3	1:B:53:CYS:HB3	1.99	0.43
1:A:471:ILE:O	1:A:472:ALA:HB2	2.18	0.43
1:B:124:LEU:HD11	1:B:130:GLU:HB2	1.99	0.43
1:A:46:GLY:O	1:A:50:ASN:HB2	2.18	0.43
1:A:105:ILE:HA	1:A:108:LEU:HB2	2.01	0.43
1:B:339:ARG:HH21	1:B:346:GLN:NE2	2.16	0.43
1:B:339:ARG:NH2	1:B:346:GLN:HE22	2.17	0.43
1:A:442:ASP:O	1:A:446:MET:HG3	2.19	0.43
1:B:120:HIS:ND1	1:B:120:HIS:C	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:SER:HB3	1:A:202:LEU:HD21	2.01	0.43
1:B:159:PRO:HB3	1:B:245:THR:O	2.18	0.43
1:A:371:THR:O	1:A:375:GLU:HG3	2.18	0.43
1:A:438:THR:HG22	1:A:442:ASP:CB	2.48	0.43
1:A:85:ILE:HG12	1:A:202:LEU:HD13	2.01	0.42
1:A:436:PHE:HZ	1:B:438:THR:CG2	2.28	0.42
1:A:156:GLU:HB2	1:A:279:ARG:HH22	1.84	0.42
1:B:85:ILE:HG12	1:B:202:LEU:CD1	2.48	0.42
1:B:321:ARG:H	1:B:321:ARG:HG3	1.70	0.42
1:A:400:GLY:HA3	1:A:419:ILE:O	2.19	0.42
1:B:176:PHE:CZ	1:B:271:LYS:HG2	2.54	0.42
1:A:306:CYS:SG	1:A:321:ARG:NH2	2.93	0.42
1:B:25:LEU:HG	1:B:341:ALA:CB	2.49	0.42
1:B:402:VAL:HG12	1:B:403:LYS:N	2.34	0.42
1:B:455:GLU:O	1:B:458:HIS:HB3	2.19	0.42
1:B:443:LEU:HA	1:B:443:LEU:HD23	1.76	0.42
1:A:28:LYS:NZ	1:A:29:THR:H	2.17	0.42
1:A:191:ILE:HG22	1:A:195:LEU:HD23	2.01	0.42
1:A:331:GLU:HB3	1:A:347:MET:SD	2.60	0.42
1:A:191:ILE:O	1:A:195:LEU:HD23	2.20	0.41
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.84	0.41
1:B:49:LEU:O	1:B:49:LEU:HG	2.20	0.41
1:A:197:SER:O	1:A:201:ARG:HD3	2.20	0.41
1:A:421:PRO:HB2	1:A:453:LEU:CD1	2.49	0.41
1:B:383:THR:HG23	1:B:401:LEU:HD12	2.03	0.41
1:A:69:ALA:HA	1:A:73:PHE:CG	2.54	0.41
1:B:51:VAL:HG11	1:B:171:THR:HG23	2.02	0.41
1:B:307:LYS:HG2	1:B:314:PHE:CE1	2.52	0.41
1:B:389:SER:HB3	1:B:392:ALA:HB3	2.02	0.41
1:A:270:ASP:O	1:A:271:LYS:HD2	2.21	0.41
1:A:307:LYS:HG2	1:A:314:PHE:CE1	2.56	0.41
1:A:410:THR:HG21	1:A:412:ARG:NH2	2.35	0.41
1:B:256:VAL:O	1:B:266:LYS:HA	2.20	0.41
1:A:47:THR:O	1:A:52:GLY:N	2.54	0.41
1:A:21:ARG:HH11	1:A:21:ARG:HD3	1.72	0.41
1:A:256:VAL:O	1:A:266:LYS:HA	2.21	0.41
1:B:152:SER:HB3	1:B:318:ASP:HB3	2.03	0.40
1:B:449:SER:HB2	1:B:452:THR:HG21	2.03	0.40
1:A:432:ILE:HD12	1:B:429:GLN:HB3	2.02	0.40
1:A:124:LEU:HD23	1:A:287:ALA:HB2	2.03	0.40
1:A:389:SER:O	1:A:393:MET:HE3	2.22	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	470/477 (98%)	439 (93%)	27 (6%)	4 (1%)	14	41
1	B	470/477 (98%)	436 (93%)	27 (6%)	7 (2%)	8	28
All	All	940/954 (98%)	875 (93%)	54 (6%)	11 (1%)	10	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	THR
1	B	283	THR
1	A	37	GLY
1	A	82	GLY
1	B	82	GLY
1	B	288	ALA
1	B	37	GLY
1	A	471	ILE
1	B	53	CYS
1	B	471	ILE
1	B	133	GLY

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	349/365 (96%)	302 (86%)	47 (14%)	4	13
1	B	349/365 (96%)	297 (85%)	52 (15%)	3	10
All	All	698/730 (96%)	599 (86%)	99 (14%)	3	12

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	21	ARG
1	A	25	LEU
1	A	28	LYS
1	A	57	LYS
1	A	79	GLU
1	A	88	PRO
1	A	96	ASN
1	A	101	LEU
1	A	102	THR
1	A	105	ILE
1	A	107	THR
1	A	108	LEU
1	A	109	PHE
1	A	155	VAL
1	A	168	VAL
1	A	182	LYS
1	A	195	LEU
1	A	201	ARG
1	A	202	LEU
1	A	222	GLN
1	A	236	LEU
1	A	254	VAL
1	A	262	ASN
1	A	265	GLN
1	A	282	THR
1	A	283	THR
1	A	307	LYS
1	A	309	SER
1	A	310	VAL
1	A	316	ILE
1	A	319	VAL
1	A	321	ARG
1	A	330	SER
1	A	352	ILE

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Mol	Chain	Res	Type
1	A	358	THR
1	A	368	THR
1	A	370	GLN
1	A	381	VAL
1	A	383	THR
1	A	391	ARG
1	A	418	VAL
1	A	419	ILE
1	A	426	LEU
1	A	438	THR
1	A	462	LEU
1	A	471	ILE
1	B	6	VAL
1	B	16	TYR
1	B	21	ARG
1	B	25	LEU
1	B	28	LYS
1	B	57	LYS
1	B	73	PHE
1	B	79	GLU
1	B	88	PRO
1	B	96	ASN
1	B	101	LEU
1	B	102	THR
1	B	105	ILE
1	B	107	THR
1	B	108	LEU
1	B	155	VAL
1	B	168	VAL
1	B	177	GLN
1	B	182	LYS
1	B	195	LEU
1	B	201	ARG
1	B	202	LEU
1	B	222	GLN
1	B	254	VAL
1	B	262	ASN
1	B	265	GLN
1	B	282	THR
1	B	283	THR
1	B	307	LYS
1	B	309	SER

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Mol	Chain	Res	Type
1	B	310	VAL
1	B	319	VAL
1	B	321	ARG
1	B	327	HIS
1	B	330	SER
1	B	344	LYS
1	B	347	MET
1	B	352	ILE
1	B	354	SER
1	B	358	THR
1	B	368	THR
1	B	370	GLN
1	B	381	VAL
1	B	383	THR
1	B	398	THR
1	B	418	VAL
1	B	419	ILE
1	B	426	LEU
1	B	438	THR
1	B	439	SER
1	B	462	LEU
1	B	471	ILE

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	2	GLN
1	A	100	ASN
1	A	112	ASN
1	A	120	HIS
1	A	145	ASN
1	A	222	GLN
1	A	234	GLN
1	A	262	ASN
1	A	346	GLN
1	A	417	HIS
1	A	429	GLN
1	A	458	HIS
1	A	465	ASN
1	B	50	ASN
1	B	120	HIS
1	B	145	ASN

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Mol	Chain	Res	Type
1	B	222	GLN
1	B	262	ASN
1	B	346	GLN
1	B	417	HIS
1	B	429	GLN
1	B	458	HIS
1	B	465	ASN

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 ⓘ

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	1.26	6 (10%)	85,89,89	2.05	26 (30%)
2	FAD	A	480	-	58,58,58	1.26	7 (12%)	85,89,89	2.03	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	B	480	-	-	1/34/50/50	0/6/6/6
2	FAD	A	480	-	-	0/34/50/50	0/6/6/6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	480	FAD	C5A-N7A	-3.82	1.32	1.39
2	B	480	FAD	C1'-C2'	3.61	1.57	1.52
2	A	480	FAD	C5X-N5	-3.52	1.33	1.39
2	B	480	FAD	C5A-N7A	-3.45	1.32	1.39
2	B	480	FAD	C5X-N5	-3.27	1.33	1.39
2	B	480	FAD	C9A-N10	-3.14	1.35	1.41
2	A	480	FAD	C9A-N10	-2.55	1.36	1.41
2	A	480	FAD	C10-N10	-2.53	1.31	1.37
2	A	480	FAD	C8A-N9A	-2.20	1.33	1.37
2	A	480	FAD	C1'-N10	-2.14	1.42	1.47
2	B	480	FAD	C10-N10	-2.12	1.32	1.37
2	B	480	FAD	C4A-N9A	-2.08	1.33	1.37
2	A	480	FAD	C4A-N9A	-2.06	1.33	1.37

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	480	FAD	C5A-C4A-N3A	-7.27	116.71	126.72
2	B	480	FAD	N3A-C4A-N9A	6.36	137.98	127.17
2	B	480	FAD	C5A-C4A-N3A	-6.33	118.00	126.72
2	A	480	FAD	N3A-C4A-N9A	6.09	137.53	127.17
2	A	480	FAD	C6A-C5A-C4A	5.67	124.92	117.18
2	B	480	FAD	C9-C9A-N10	5.27	128.94	121.85
2	A	480	FAD	C6A-C5A-N7A	-5.09	122.28	132.09
2	B	480	FAD	C6A-C5A-C4A	5.09	124.12	117.18
2	A	480	FAD	C9-C9A-N10	4.88	128.41	121.85
2	B	480	FAD	C6A-C5A-N7A	-4.72	122.99	132.09
2	A	480	FAD	C4-N3-C2	-4.51	117.64	125.64
2	B	480	FAD	C4-N3-C2	-4.43	117.78	125.64
2	B	480	FAD	N3A-C2A-N1A	-3.60	123.13	128.58
2	B	480	FAD	C10-N1-C2	3.22	123.81	116.85
2	A	480	FAD	O2-C2-N1	-2.91	116.97	121.80
2	B	480	FAD	C9-C9A-C5X	-2.88	114.94	120.03
2	B	480	FAD	C4X-C10-N1	-2.84	117.62	124.59
2	A	480	FAD	C2A-N3A-C4A	2.78	118.62	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	480	FAD	C9-C9A-C5X	-2.77	115.13	120.03
2	A	480	FAD	N3A-C2A-N1A	-2.74	124.44	128.58
2	B	480	FAD	C4A-N9A-C8A	2.67	108.54	105.74
2	B	480	FAD	C4X-C4-N3	2.63	119.94	113.25
2	A	480	FAD	C10-C4X-N5	-2.63	119.45	124.81
2	B	480	FAD	C2A-N3A-C4A	2.61	118.22	111.83
2	A	480	FAD	C10-N1-C2	2.61	122.49	116.85
2	B	480	FAD	C5X-C9A-N10	-2.59	115.63	117.97
2	A	480	FAD	C4X-C10-N1	-2.52	118.40	124.59
2	B	480	FAD	C10-C4X-N5	-2.38	119.94	124.81
2	A	480	FAD	O2A-PA-O3P	-2.38	100.84	107.27
2	B	480	FAD	C1'-C2'-C3'	-2.38	103.21	109.66
2	B	480	FAD	C1'-N10-C9A	-2.36	116.04	120.63
2	A	480	FAD	C4X-C4-N3	2.35	119.24	113.25
2	B	480	FAD	O2'-C2'-C1'	2.33	119.79	110.20
2	B	480	FAD	N6A-C6A-N1A	2.30	123.51	118.38
2	B	480	FAD	C2A-N1A-C6A	2.25	122.43	118.73
2	B	480	FAD	C9A-N10-C10	2.24	124.16	120.75
2	B	480	FAD	O4-C4-C4X	-2.23	120.66	126.53
2	A	480	FAD	C4-C4X-C10	2.19	120.69	116.93
2	B	480	FAD	C9A-C9-C8	2.19	123.62	119.22
2	A	480	FAD	O4-C4-C4X	-2.17	120.81	126.53
2	A	480	FAD	C1'-N10-C9A	-2.09	116.57	120.63
2	B	480	FAD	N10-C10-N1	2.07	124.62	118.51
2	B	480	FAD	N9A-C8A-N7A	-2.07	111.00	113.94
2	B	480	FAD	C4A-C5A-N7A	2.02	112.89	110.58

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	480	FAD	O4B-C4B-C5B-O5B

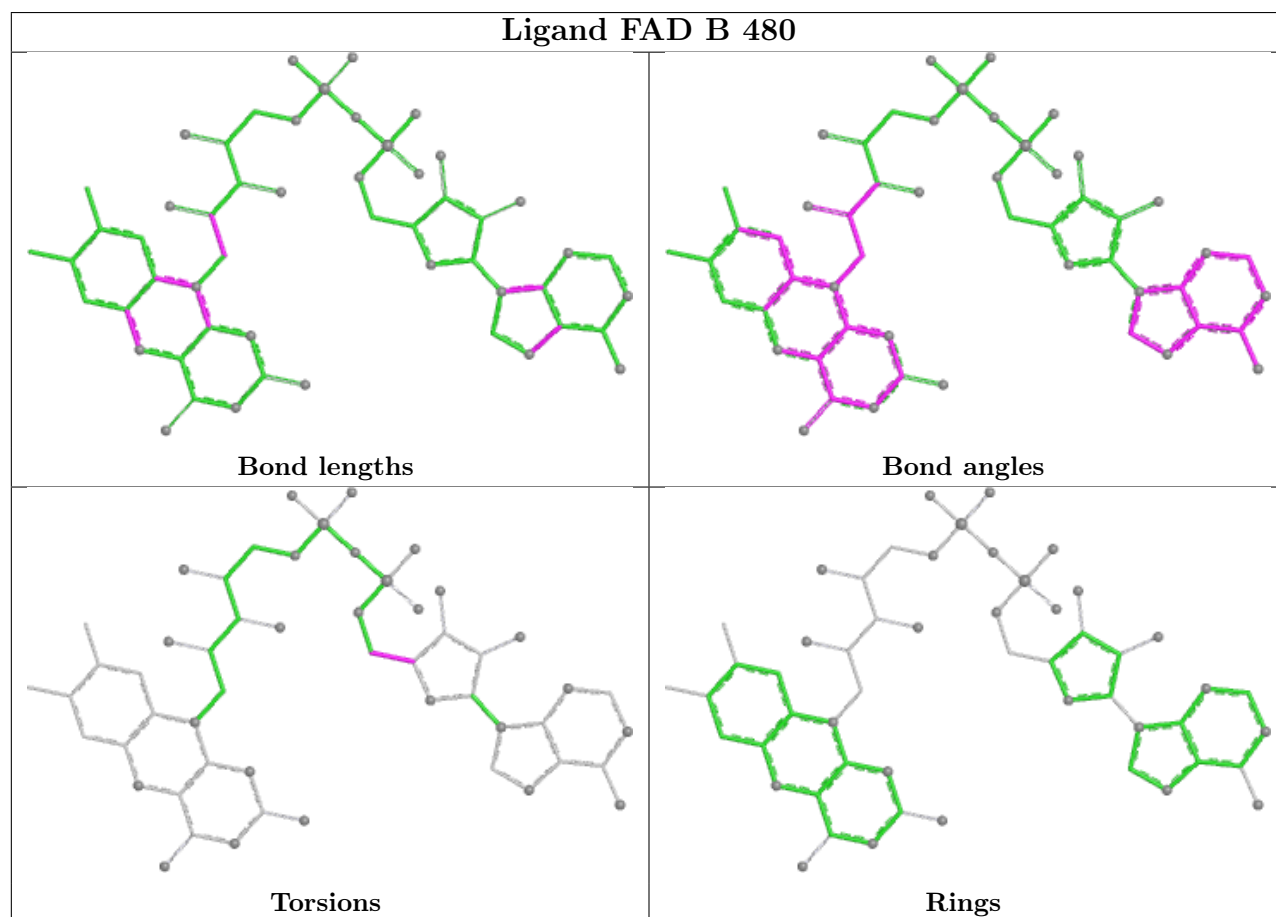
There are no ring outliers.

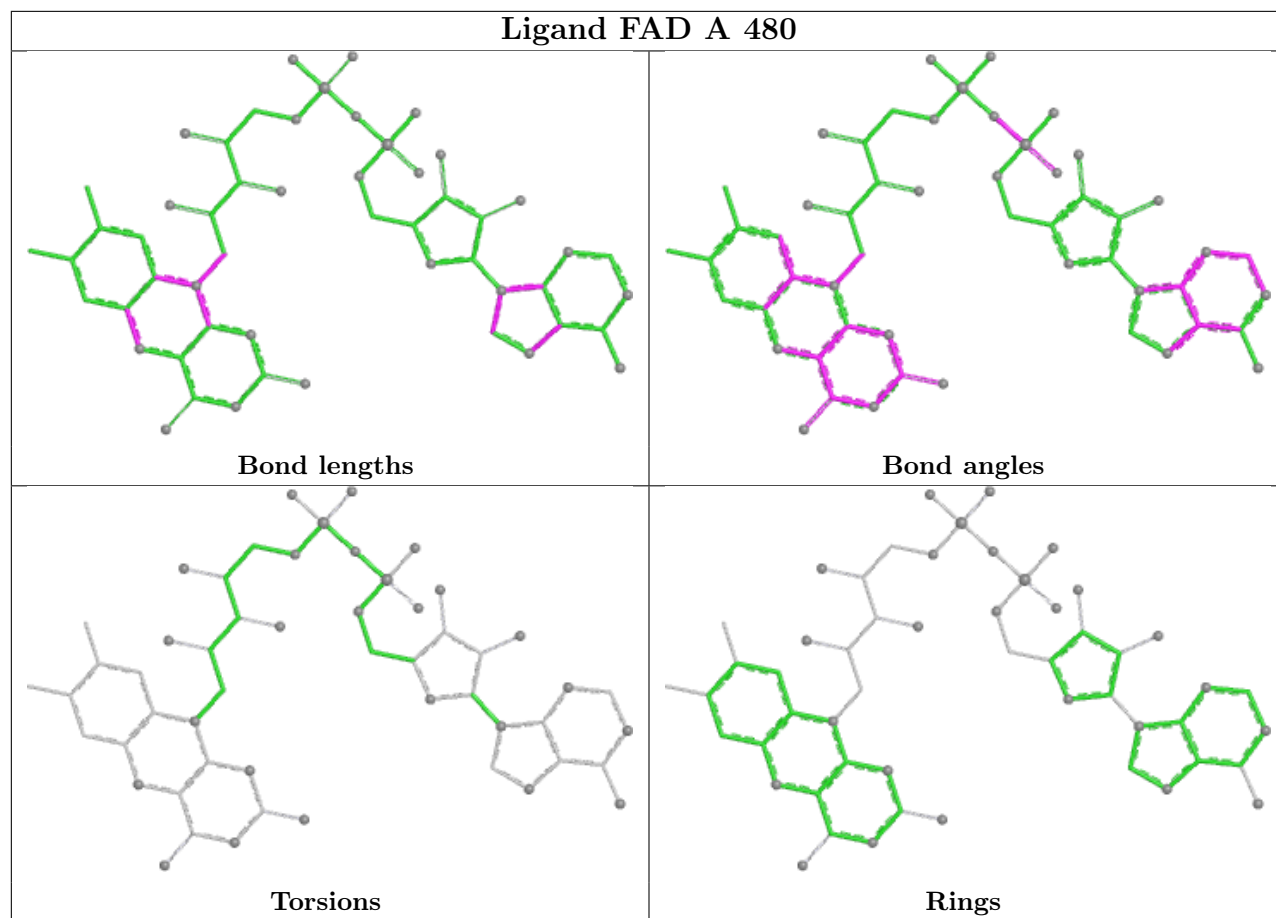
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	480	FAD	1	0
2	A	480	FAD	1	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	472/477 (98%)	-0.73	2 (0%) 88 84	6, 26, 63, 89	0
1	B	472/477 (98%)	-0.67	3 (0%) 85 80	6, 28, 63, 90	0
All	All	944/954 (98%)	-0.70	5 (0%) 87 82	6, 27, 63, 90	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	262	ASN	4.5
1	A	262	ASN	3.8
1	B	472	ALA	2.6
1	B	263	GLY	2.3
1	A	472	ALA	2.1

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](#)

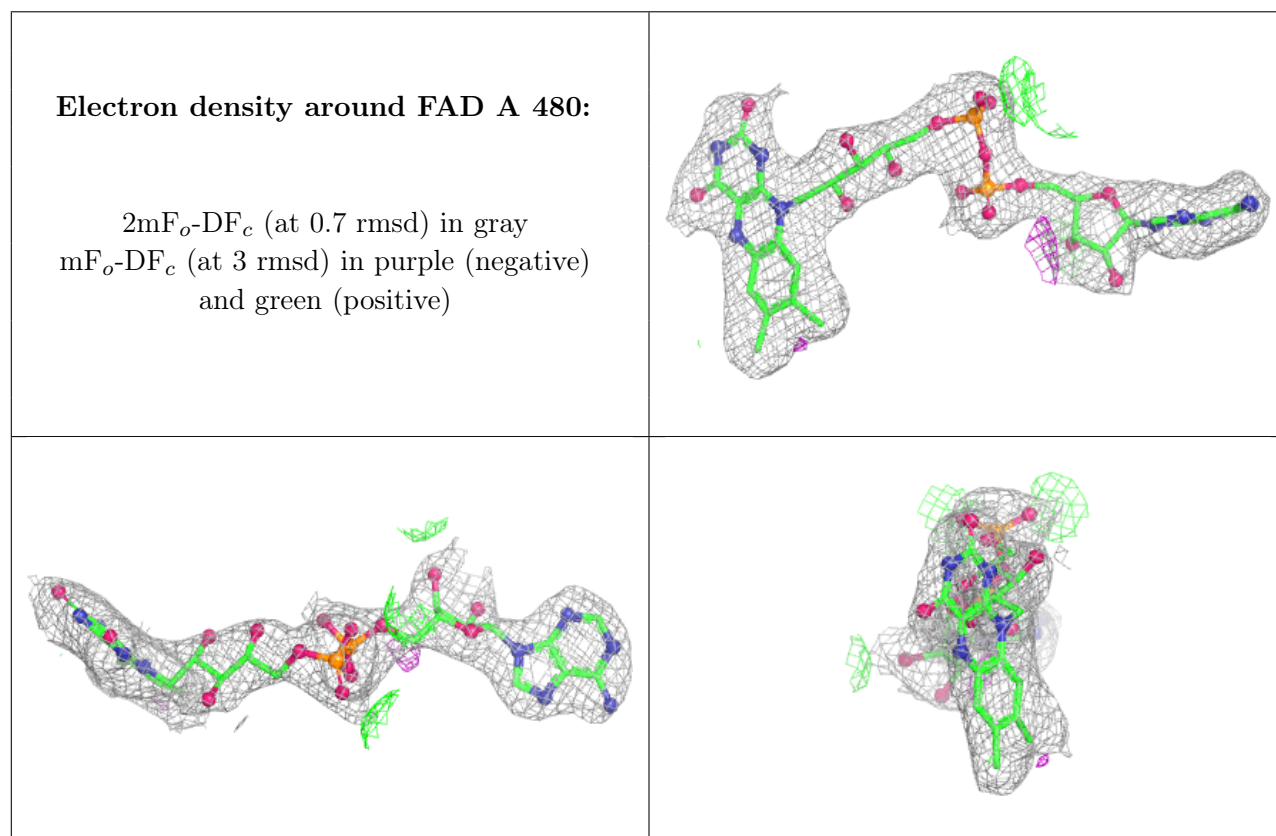
There are no oligosaccharides in this entry.

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.

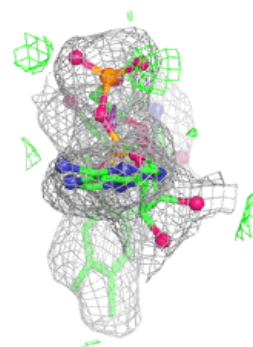
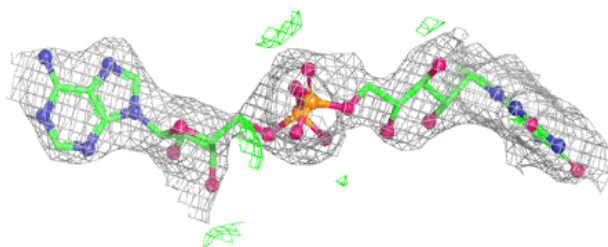
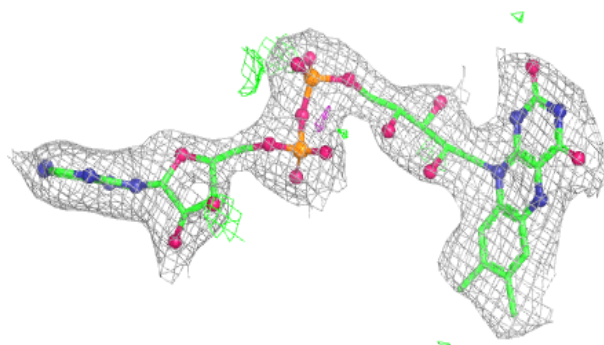
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	A	480	53/53	0.97	0.06	9,23,30,32	0
2	FAD	B	480	53/53	0.97	0.06	10,26,35,37	0

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 480:

$2mF_o - DF_c$ (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.