



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:20 PM UTC

PDB ID : 1OJT / pdb_00001ojt
Title : STRUCTURE OF DIHYDROLIPOAMIDE DEHYDROGENASE
Authors : Li De La Sierra, I.; Prange, T.; Pernot, L.
Deposited on : 1996-09-06
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	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

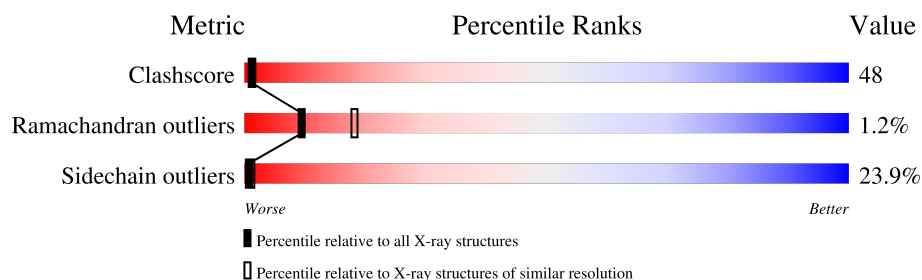
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)

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	482	26% 41% 25% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	A	600	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3724 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 SURFACE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	482	3556	2243	616	677	20	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	498	ALA	GLY	conflict	UNP Q51225

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



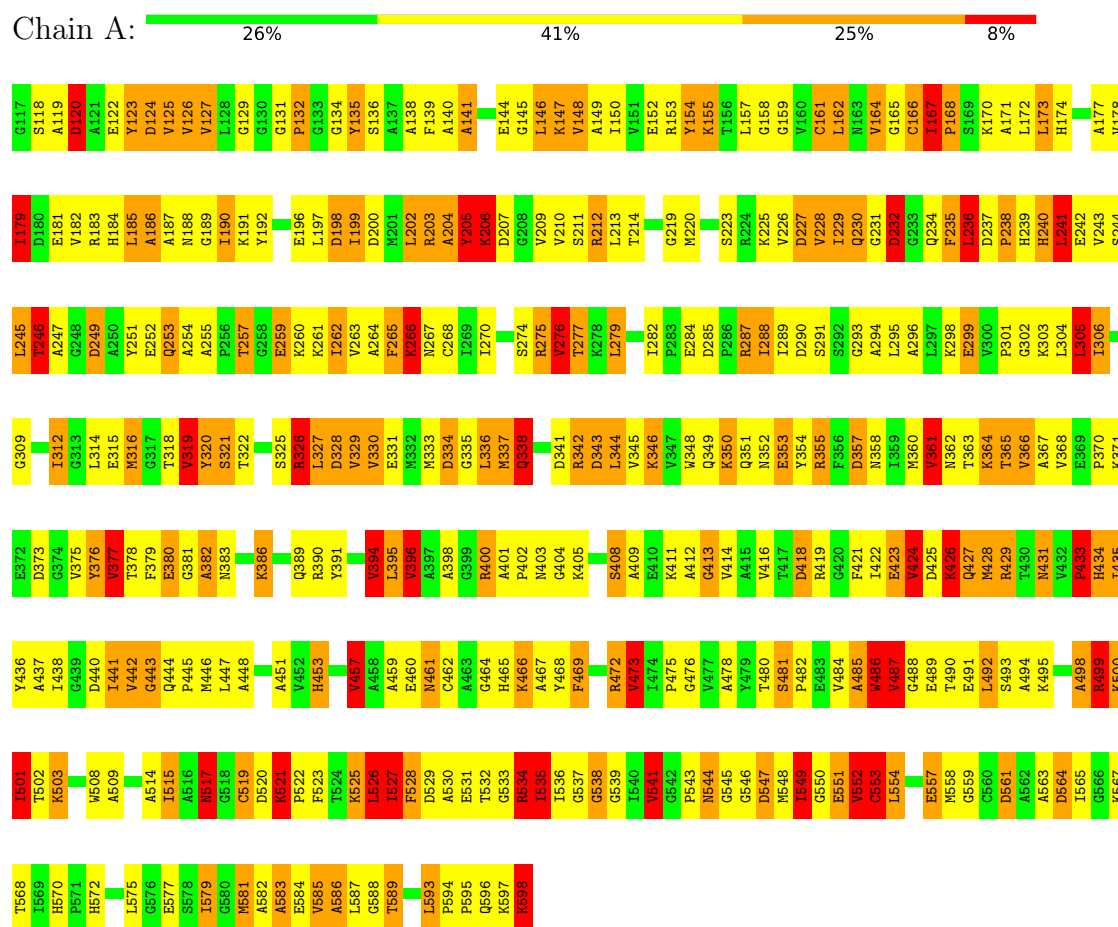
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total 115	O 115	0	0

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: SURFACE PROTEIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	138.05 Å 138.05 Å 79.77 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 2.75	Depositor
% Data completeness (in resolution range)	(Not available) (18.00-2.75)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.173 , 0.232	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3724	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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	1.74	24/3621 (0.7%)	2.60	295/4907 (6.0%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	538	GLY	CA-C	7.28	1.58	1.51
1	A	561	ASP	CA-C	6.11	1.60	1.52
1	A	552	VAL	C-N	6.02	1.42	1.33
1	A	167	ILE	C-O	6.00	1.29	1.24
1	A	158	GLY	N-CA	5.93	1.53	1.45
1	A	597	LYS	N-CA	5.87	1.53	1.46
1	A	476	GLY	N-CA	5.79	1.52	1.45
1	A	535	ILE	CA-C	5.76	1.59	1.52
1	A	551	GLU	N-CA	5.71	1.53	1.46
1	A	447	LEU	C-O	5.60	1.30	1.23
1	A	161	CYS	C-O	5.58	1.30	1.24
1	A	209	VAL	N-CA	5.57	1.53	1.46
1	A	368	VAL	CA-C	5.49	1.59	1.52
1	A	598	LYS	C-O	5.43	1.34	1.23
1	A	190	ILE	N-CA	5.35	1.53	1.46
1	A	203	ARG	NE-CZ	5.30	1.38	1.33
1	A	190	ILE	CA-C	5.27	1.59	1.52
1	A	228	VAL	N-CA	5.24	1.52	1.46
1	A	460	GLU	N-CA	5.21	1.52	1.46
1	A	443	GLY	N-CA	5.15	1.50	1.45
1	A	453	HIS	C-O	5.13	1.30	1.24
1	A	597	LYS	C-N	5.10	1.40	1.33
1	A	473	VAL	N-CA	5.09	1.52	1.46
1	A	480	THR	C-N	5.08	1.38	1.33

All (295) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	501	ILE	N-CA-CB	-13.62	95.03	112.60
1	A	424	VAL	N-CA-CB	-13.59	96.70	112.32
1	A	487	VAL	CB-CA-C	-12.95	93.14	111.40
1	A	541	VAL	CB-CA-C	-12.34	94.08	110.98
1	A	167	ILE	N-CA-CB	-11.48	101.50	110.45
1	A	287	ARG	CD-NE-CZ	-11.28	108.61	124.40
1	A	190	ILE	N-CA-CB	11.03	125.57	111.67
1	A	343	ASP	CA-CB-CG	10.65	123.25	112.60
1	A	240	HIS	CA-CB-CG	-10.47	103.33	113.80
1	A	519	CYS	CA-C-O	-10.25	110.30	121.78
1	A	266	LYS	N-CA-C	-10.08	99.98	110.97
1	A	473	VAL	N-CA-CB	-10.05	94.97	111.45
1	A	541	VAL	N-CA-CB	10.05	122.97	111.21
1	A	541	VAL	CA-C-O	-9.94	109.75	120.59
1	A	548	MET	CA-C-O	-9.85	108.28	119.41
1	A	227	ASP	CA-C-N	-9.83	109.69	122.37
1	A	227	ASP	C-N-CA	-9.83	109.69	122.37
1	A	544	ASN	CA-CB-CG	-9.66	102.94	112.60
1	A	326	ARG	N-CA-C	-9.51	94.17	109.76
1	A	535	ILE	N-CA-CB	9.49	124.94	110.13
1	A	365	THR	CA-C-N	-9.44	111.39	122.63
1	A	365	THR	C-N-CA	-9.44	111.39	122.63
1	A	465	HIS	CA-C-O	-9.34	110.73	121.47
1	A	179	ILE	CA-C-O	-9.32	110.97	120.85
1	A	355	ARG	NE-CZ-NH2	-9.31	110.82	119.20
1	A	267	ASN	OD1-CG-ND2	9.20	131.80	122.60
1	A	236	LEU	CA-C-O	9.17	131.77	120.31
1	A	534	ARG	CA-C-O	-9.08	111.03	121.47
1	A	557	GLU	CA-C-O	-9.03	111.52	121.00
1	A	535	ILE	CB-CA-C	-8.96	97.64	111.26
1	A	253	GLN	CB-CG-CD	8.79	127.55	112.60
1	A	253	GLN	N-CA-CB	8.76	127.03	110.90
1	A	469	PHE	N-CA-C	-8.74	94.64	108.63
1	A	209	VAL	N-CA-C	-8.70	102.35	110.53
1	A	418	ASP	CA-CB-CG	-8.68	103.92	112.60
1	A	365	THR	N-CA-CB	8.63	123.75	109.94
1	A	487	VAL	N-CA-CB	8.46	124.92	110.96
1	A	423	GLU	N-CA-CB	8.45	122.47	110.04
1	A	461	ASN	CA-CB-CG	-8.25	104.35	112.60
1	A	435	ILE	CA-C-O	8.24	129.54	120.48
1	A	551	GLU	CA-C-O	-8.18	111.16	120.24
1	A	253	GLN	OE1-CD-NE2	-8.15	114.45	122.60
1	A	167	ILE	O-C-N	-8.08	115.25	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	598	LYS	CA-C-O	-8.02	107.17	120.80
1	A	287	ARG	NE-CZ-NH1	-7.98	113.52	121.50
1	A	501	ILE	CB-CA-C	7.93	122.06	111.19
1	A	547	ASP	CA-CB-CG	-7.91	104.69	112.60
1	A	377	VAL	CA-C-O	7.85	128.68	120.36
1	A	158	GLY	N-CA-C	-7.70	104.66	114.37
1	A	517	ASN	CA-CB-CG	-7.67	104.93	112.60
1	A	596	GLN	CB-CG-CD	7.67	125.64	112.60
1	A	167	ILE	N-CA-C	7.67	121.55	112.35
1	A	451	ALA	CA-C-N	-7.66	109.97	120.46
1	A	451	ALA	C-N-CA	-7.66	109.97	120.46
1	A	270	ILE	CA-C-O	-7.63	111.72	120.95
1	A	334	ASP	CA-CB-CG	-7.58	105.02	112.60
1	A	328	ASP	N-CA-C	-7.57	97.53	109.50
1	A	469	PHE	CA-C-O	-7.55	112.33	121.02
1	A	203	ARG	NH1-CZ-NH2	7.54	129.10	119.30
1	A	357	ASP	N-CA-C	-7.48	101.27	112.04
1	A	478	ALA	N-CA-C	-7.48	97.06	108.96
1	A	593	LEU	O-C-N	7.44	126.47	121.71
1	A	275	ARG	NE-CZ-NH2	-7.43	112.51	119.20
1	A	581	MET	CA-CB-CG	-7.40	99.30	114.10
1	A	242	GLU	CA-C-O	-7.36	112.89	120.54
1	A	253	GLN	CB-CA-C	-7.33	101.61	112.09
1	A	226	VAL	CA-C-O	-7.33	111.33	121.51
1	A	171	ALA	CA-C-O	7.32	128.18	120.42
1	A	424	VAL	CB-CA-C	7.30	121.58	110.91
1	A	575	LEU	CA-C-O	7.30	128.90	120.00
1	A	515	ILE	N-CA-C	-7.30	103.22	110.30
1	A	434	HIS	O-C-N	7.28	130.92	122.25
1	A	589	THR	N-CA-CB	-7.24	99.50	110.73
1	A	412	ALA	N-CA-C	-7.17	104.57	113.38
1	A	469	PHE	CA-CB-CG	7.11	120.91	113.80
1	A	487	VAL	O-C-N	7.11	130.06	122.67
1	A	227	ASP	CA-CB-CG	7.07	119.67	112.60
1	A	561	ASP	N-CA-CB	7.06	121.64	111.05
1	A	266	LYS	CA-C-O	7.06	128.41	121.00
1	A	521	LYS	CA-C-O	7.05	129.82	120.16
1	A	585	VAL	N-CA-C	-7.04	103.44	110.62
1	A	257	THR	CA-CB-OG1	-7.02	99.06	109.60
1	A	154	TYR	CA-C-O	-7.02	113.10	121.60
1	A	191	LYS	N-CA-C	7.00	120.31	108.90
1	A	427	GLN	CA-C-O	6.99	127.53	119.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	GLN	CA-C-O	-6.98	112.72	120.60
1	A	188	ASN	N-CA-C	-6.96	104.79	112.72
1	A	345	VAL	O-C-N	6.94	128.60	121.87
1	A	534	ARG	NE-CZ-NH2	-6.94	112.96	119.20
1	A	328	ASP	CA-C-O	-6.93	113.00	121.11
1	A	154	TYR	CA-C-N	-6.92	110.28	122.26
1	A	154	TYR	C-N-CA	-6.92	110.28	122.26
1	A	187	ALA	CA-C-O	-6.92	111.12	119.49
1	A	120	ASP	CA-CB-CG	6.89	119.49	112.60
1	A	123	TYR	CA-C-N	6.88	129.74	120.65
1	A	123	TYR	C-N-CA	6.88	129.74	120.65
1	A	472	ARG	CA-C-N	-6.88	112.80	122.71
1	A	472	ARG	C-N-CA	-6.88	112.80	122.71
1	A	136	SER	N-CA-C	-6.87	103.72	111.14
1	A	441	ILE	CA-C-N	6.83	130.51	120.74
1	A	441	ILE	C-N-CA	6.83	130.51	120.74
1	A	290	ASP	N-CA-C	-6.82	99.18	109.96
1	A	270	ILE	CB-CA-C	-6.82	102.20	111.33
1	A	230	GLN	OE1-CD-NE2	6.79	129.38	122.60
1	A	204	ALA	CA-C-O	-6.77	112.18	119.97
1	A	499	ARG	N-CA-C	-6.75	100.98	110.50
1	A	232	ASP	CA-CB-CG	-6.73	105.87	112.60
1	A	490	THR	N-CA-CB	6.73	122.10	111.20
1	A	380	GLU	CA-C-O	-6.72	113.44	120.70
1	A	203	ARG	CG-CD-NE	6.67	126.67	112.00
1	A	460	GLU	CB-CG-CD	-6.65	101.29	112.60
1	A	475	PRO	N-CA-C	6.62	121.58	111.19
1	A	368	VAL	N-CA-CB	6.60	122.12	111.23
1	A	598	LYS	CA-CB-CG	-6.60	100.91	114.10
1	A	203	ARG	NE-CZ-NH1	-6.57	114.93	121.50
1	A	219	GLY	O-C-N	6.57	128.50	122.19
1	A	473	VAL	CB-CA-C	6.57	122.08	110.71
1	A	124	ASP	CA-C-O	6.57	127.89	121.00
1	A	245	LEU	CA-C-O	6.53	129.85	120.51
1	A	190	ILE	CA-C-N	-6.53	113.79	122.99
1	A	190	ILE	C-N-CA	-6.53	113.79	122.99
1	A	262	ILE	N-CA-CB	6.52	119.68	111.46
1	A	232	ASP	CB-CA-C	6.52	120.46	109.84
1	A	394	VAL	O-C-N	6.50	130.22	123.20
1	A	409	ALA	O-C-N	6.50	129.82	122.22
1	A	246	THR	N-CA-CB	-6.49	99.57	111.37
1	A	205	TYR	O-C-N	6.48	129.53	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	HIS	CA-CB-CG	-6.43	107.37	113.80
1	A	538	GLY	N-CA-C	-6.41	101.01	110.87
1	A	326	ARG	N-CA-CB	6.38	121.06	110.52
1	A	585	VAL	CB-CA-C	6.36	120.73	112.14
1	A	579	ILE	N-CA-C	-6.34	104.34	110.42
1	A	266	LYS	N-CA-CB	6.33	119.16	109.91
1	A	277	THR	CA-C-O	-6.33	113.42	120.70
1	A	190	ILE	N-CA-C	-6.30	98.05	107.37
1	A	485	ALA	CA-C-O	-6.29	114.05	120.71
1	A	543	PRO	CA-C-O	-6.26	114.28	121.36
1	A	206	LYS	CA-C-O	6.25	127.56	121.00
1	A	305	LEU	N-CA-C	-6.24	101.24	110.48
1	A	279	LEU	N-CA-C	-6.23	102.21	109.93
1	A	564	ASP	CA-C-O	6.23	127.11	120.70
1	A	552	VAL	CA-C-O	6.22	127.73	119.70
1	A	394	VAL	N-CA-CB	6.19	120.56	111.52
1	A	196	GLU	N-CA-C	-6.19	99.18	109.46
1	A	265	PHE	N-CA-C	6.19	119.59	109.06
1	A	554	LEU	CA-C-O	6.18	127.08	119.97
1	A	186	ALA	O-C-N	6.14	128.40	122.07
1	A	197	LEU	CB-CA-C	-6.13	100.69	110.81
1	A	498	ALA	CA-C-O	6.12	128.39	120.81
1	A	183	ARG	N-CA-C	-6.11	104.53	111.07
1	A	253	GLN	O-C-N	6.09	132.13	122.81
1	A	289	ILE	N-CA-CB	-6.09	102.24	112.47
1	A	396	VAL	N-CA-CB	6.07	118.78	111.31
1	A	365	THR	CB-CA-C	-6.06	100.66	110.77
1	A	168	PRO	N-CA-C	-6.04	105.30	113.40
1	A	355	ARG	NH1-CZ-NH2	6.03	127.14	119.30
1	A	361	VAL	CA-C-O	-6.01	115.95	121.72
1	A	168	PRO	CA-C-N	-6.01	112.63	120.44
1	A	168	PRO	C-N-CA	-6.01	112.63	120.44
1	A	302	GLY	N-CA-C	-5.99	105.11	112.77
1	A	210	VAL	N-CA-C	5.91	116.56	110.36
1	A	575	LEU	N-CA-C	-5.90	104.25	112.45
1	A	472	ARG	CD-NE-CZ	5.89	132.65	124.40
1	A	275	ARG	N-CA-CB	-5.88	101.84	111.66
1	A	150	ILE	N-CA-CB	5.87	119.23	111.25
1	A	564	ASP	CA-CB-CG	-5.86	106.74	112.60
1	A	447	LEU	O-C-N	-5.86	116.22	123.36
1	A	179	ILE	CB-CG1-CD1	-5.85	101.51	113.80
1	A	187	ALA	CA-C-N	-5.84	113.32	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	ALA	C-N-CA	-5.84	113.32	122.73
1	A	382	ALA	CA-C-O	-5.83	114.81	121.40
1	A	299	GLU	CB-CG-CD	-5.83	102.69	112.60
1	A	404	GLY	CA-C-O	5.81	126.73	120.75
1	A	275	ARG	NH1-CZ-NH2	5.80	126.84	119.30
1	A	538	GLY	CA-C-O	-5.80	115.84	121.06
1	A	185	LEU	N-CA-C	5.79	123.14	110.80
1	A	371	LYS	CA-C-O	-5.79	114.86	121.58
1	A	457	VAL	CA-C-O	-5.78	114.63	121.05
1	A	527	ILE	O-C-N	5.76	129.40	123.18
1	A	197	LEU	CA-C-O	-5.75	114.42	120.58
1	A	136	SER	O-C-N	5.71	128.26	122.09
1	A	145	GLY	N-CA-C	-5.70	107.45	115.32
1	A	162	LEU	CA-C-N	5.70	133.79	121.64
1	A	162	LEU	C-N-CA	5.70	133.79	121.64
1	A	257	THR	N-CA-CB	-5.69	100.44	110.39
1	A	583	ALA	CA-C-O	-5.67	115.04	121.00
1	A	196	GLU	N-CA-CB	5.67	119.51	110.16
1	A	136	SER	CA-C-O	-5.65	114.88	120.70
1	A	253	GLN	CG-CD-NE2	5.64	124.86	116.40
1	A	304	LEU	CA-C-O	5.64	126.22	120.24
1	A	486	TRP	N-CA-CB	5.63	120.45	111.56
1	A	326	ARG	CA-C-O	-5.62	114.56	120.80
1	A	338	GLN	CA-C-N	-5.62	116.75	123.44
1	A	338	GLN	C-N-CA	-5.62	116.75	123.44
1	A	546	GLY	CA-C-N	-5.62	111.31	121.14
1	A	546	GLY	C-N-CA	-5.62	111.31	121.14
1	A	203	ARG	CA-C-O	5.61	127.20	120.92
1	A	319	VAL	O-C-N	5.60	127.73	121.90
1	A	475	PRO	CB-CA-C	-5.59	103.77	111.21
1	A	229	ILE	CA-C-O	-5.58	114.56	120.53
1	A	501	ILE	O-C-N	-5.58	117.11	122.97
1	A	267	ASN	CA-CB-CG	-5.56	107.04	112.60
1	A	268	CYS	CA-C-N	-5.55	115.33	123.10
1	A	268	CYS	C-N-CA	-5.55	115.33	123.10
1	A	226	VAL	CA-C-N	-5.52	115.43	122.77
1	A	226	VAL	C-N-CA	-5.52	115.43	122.77
1	A	539	GLY	N-CA-C	-5.52	100.11	113.18
1	A	468	TYR	CA-C-N	-5.51	112.71	122.07
1	A	468	TYR	C-N-CA	-5.51	112.71	122.07
1	A	467	ALA	CA-C-O	-5.50	114.76	120.70
1	A	316	MET	O-C-N	5.49	127.73	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	ILE	CA-C-N	-5.49	114.19	122.81
1	A	527	ILE	C-N-CA	-5.49	114.19	122.81
1	A	376	TYR	CA-C-N	-5.49	115.36	122.99
1	A	376	TYR	C-N-CA	-5.49	115.36	122.99
1	A	192	TYR	N-CA-CB	5.48	120.37	110.72
1	A	468	TYR	CA-CB-CG	-5.48	104.04	113.90
1	A	141	ALA	CA-C-O	5.48	126.76	120.90
1	A	135	TYR	CB-CA-C	5.47	121.43	109.99
1	A	312	ILE	CB-CA-C	-5.47	104.87	111.88
1	A	457	VAL	N-CA-CB	5.47	117.57	110.57
1	A	241	LEU	CA-C-N	-5.47	115.73	122.84
1	A	241	LEU	C-N-CA	-5.47	115.73	122.84
1	A	588	GLY	O-C-N	-5.47	115.67	122.34
1	A	198	ASP	CA-C-O	-5.46	114.94	120.84
1	A	219	GLY	CA-C-O	-5.46	115.12	120.75
1	A	320	TYR	CA-C-O	-5.45	115.10	120.82
1	A	396	VAL	O-C-N	5.45	129.52	122.77
1	A	319	VAL	N-CA-CB	5.44	117.54	110.57
1	A	134	GLY	CA-C-N	-5.44	111.63	121.14
1	A	134	GLY	C-N-CA	-5.44	111.63	121.14
1	A	228	VAL	CA-C-O	-5.42	114.59	120.71
1	A	353	GLU	CA-CB-CG	5.40	124.91	114.10
1	A	306	ILE	CA-C-N	-5.40	115.62	122.37
1	A	306	ILE	C-N-CA	-5.40	115.62	122.37
1	A	433	PRO	CA-C-N	-5.37	114.22	122.60
1	A	433	PRO	C-N-CA	-5.37	114.22	122.60
1	A	395	LEU	CA-C-N	-5.37	115.67	122.43
1	A	395	LEU	C-N-CA	-5.37	115.67	122.43
1	A	553	CYS	CB-CA-C	5.36	120.24	110.11
1	A	132	PRO	O-C-N	5.35	128.65	122.23
1	A	148	VAL	N-CA-C	5.35	117.34	108.99
1	A	528	PHE	CA-CB-CG	-5.33	108.47	113.80
1	A	179	ILE	CA-CB-CG1	5.33	119.46	110.40
1	A	305	LEU	N-CA-CB	5.33	118.38	110.29
1	A	433	PRO	CA-C-O	-5.29	111.28	119.64
1	A	586	ALA	N-CA-C	-5.29	105.41	111.07
1	A	366	VAL	CB-CA-C	5.29	118.04	111.80
1	A	526	LEU	CA-C-N	-5.28	115.77	123.06
1	A	526	LEU	C-N-CA	-5.28	115.77	123.06
1	A	528	PHE	O-C-N	5.27	130.04	123.19
1	A	322	THR	CA-CB-OG1	-5.27	101.70	109.60
1	A	235	PHE	CA-CB-CG	-5.26	108.54	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	HIS	CA-C-O	5.25	126.73	120.28
1	A	549	ILE	CB-CG1-CD1	-5.23	102.82	113.80
1	A	531	GLU	CB-CG-CD	-5.21	103.75	112.60
1	A	202	LEU	N-CA-C	-5.20	105.30	110.97
1	A	140	ALA	CA-C-O	5.20	126.25	120.90
1	A	423	GLU	CB-CA-C	-5.20	100.32	109.62
1	A	166	CYS	CA-C-N	-5.18	116.18	120.33
1	A	166	CYS	C-N-CA	-5.18	116.18	120.33
1	A	329	VAL	CA-C-N	-5.18	116.35	123.14
1	A	329	VAL	C-N-CA	-5.18	116.35	123.14
1	A	567	LYS	CA-C-N	-5.18	114.09	121.50
1	A	567	LYS	C-N-CA	-5.18	114.09	121.50
1	A	329	VAL	N-CA-C	-5.17	100.79	108.45
1	A	400	ARG	CA-CB-CG	-5.17	103.75	114.10
1	A	465	HIS	N-CA-C	-5.17	102.83	110.48
1	A	318	THR	CA-C-N	-5.17	113.95	120.56
1	A	318	THR	C-N-CA	-5.17	113.95	120.56
1	A	481	SER	CA-CB-OG	-5.15	100.80	111.10
1	A	120	ASP	N-CA-CB	5.15	121.10	111.52
1	A	126	VAL	CA-C-N	-5.15	116.31	122.90
1	A	126	VAL	C-N-CA	-5.15	116.31	122.90
1	A	413	GLY	N-CA-C	-5.14	108.52	115.21
1	A	242	GLU	CA-C-N	-5.14	116.20	122.93
1	A	242	GLU	C-N-CA	-5.14	116.20	122.93
1	A	288	ILE	N-CA-C	-5.12	99.79	107.37
1	A	528	PHE	N-CA-C	5.12	117.91	109.72
1	A	124	ASP	CA-CB-CG	-5.11	107.49	112.60
1	A	365	THR	CA-C-O	-5.09	114.85	120.60
1	A	561	ASP	N-CA-C	-5.09	102.03	109.81
1	A	242	GLU	CB-CG-CD	-5.08	103.96	112.60
1	A	466	LYS	N-CA-CB	5.08	118.70	110.42
1	A	192	TYR	CB-CA-C	-5.07	101.01	108.87
1	A	276	VAL	CA-C-O	5.07	127.00	121.13
1	A	448	ALA	N-CA-CB	-5.06	102.14	110.14
1	A	179	ILE	CB-CA-C	5.06	119.20	112.22
1	A	187	ALA	N-CA-C	-5.05	106.21	112.38
1	A	564	ASP	N-CA-C	5.05	116.60	111.14
1	A	517	ASN	CA-C-O	5.05	125.26	119.35
1	A	205	TYR	N-CA-CB	5.03	117.60	110.16
1	A	203	ARG	CD-NE-CZ	-5.00	117.39	124.40
1	A	212	ARG	CD-NE-CZ	-5.00	117.40	124.40
1	A	460	GLU	CA-C-O	-5.00	115.57	120.82

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	3556	0	3576	346	2
2	A	53	0	31	7	0
3	A	115	0	0	23	1
All	All	3724	0	3607	347	2

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 48.

All (347) 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:275:ARG:NH1	1:A:403:ASN:HD22	1.28	1.30
1:A:275:ARG:HH11	1:A:403:ASN:ND2	1.34	1.24
1:A:426:LYS:H	1:A:426:LYS:HE2	0.98	1.14
1:A:386:LYS:H	1:A:386:LYS:HD2	1.07	1.10
1:A:521:LYS:N	1:A:522:PRO:HD3	1.59	1.09
1:A:199:ILE:HD13	1:A:200:ASP:N	1.69	1.06
1:A:144:GLU:OE1	1:A:144:GLU:HA	1.52	1.05
1:A:534:ARG:HH11	1:A:559:GLY:HA2	1.22	1.03
1:A:230:GLN:HG2	1:A:246:THR:HG22	1.04	1.02
1:A:230:GLN:CG	1:A:246:THR:HG22	1.88	1.01
1:A:534:ARG:NH1	1:A:559:GLY:HA2	1.75	1.01
1:A:295:LEU:HG	1:A:316:MET:CE	1.93	0.98
1:A:521:LYS:N	1:A:522:PRO:CD	2.29	0.96
1:A:303:LYS:HG2	1:A:326:ARG:HG2	1.48	0.95
1:A:426:LYS:HE2	1:A:426:LYS:N	1.81	0.95
1:A:538:GLY:HA3	1:A:552:VAL:HG21	1.49	0.94
1:A:295:LEU:HG	1:A:316:MET:HE1	1.50	0.93
1:A:501:ILE:HD11	1:A:536:ILE:HD11	1.50	0.92
1:A:321:SER:HB3	1:A:355:ARG:NH1	1.85	0.91
1:A:453:HIS:HB3	1:A:469:PHE:HE1	1.34	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:GLN:HG2	1:A:246:THR:CG2	1.99	0.91
1:A:386:LYS:HD2	1:A:386:LYS:N	1.85	0.90
1:A:521:LYS:H	1:A:522:PRO:HD3	1.33	0.89
1:A:426:LYS:H	1:A:426:LYS:CE	1.85	0.88
1:A:521:LYS:HE2	1:A:522:PRO:HG3	1.56	0.85
1:A:331:GLU:OE2	1:A:333:MET:HG2	1.76	0.85
1:A:353:GLU:HG3	3:A:773:HOH:O	1.76	0.84
1:A:386:LYS:H	1:A:386:LYS:CD	1.90	0.84
1:A:144:GLU:OE1	1:A:144:GLU:CA	2.24	0.84
1:A:200:ASP:OD2	3:A:762:HOH:O	1.96	0.84
1:A:257:THR:HG22	1:A:259:GLU:H	1.42	0.84
1:A:501:ILE:HG12	1:A:527:ILE:HD12	1.59	0.84
1:A:508:TRP:HB2	1:A:522:PRO:O	1.79	0.83
1:A:331:GLU:HG2	1:A:335:GLY:O	1.78	0.82
1:A:509:ALA:HA	1:A:520:ASP:HB2	1.59	0.82
1:A:288:ILE:HG23	1:A:394:VAL:CG2	2.10	0.82
1:A:321:SER:HB3	1:A:355:ARG:HH11	1.42	0.82
1:A:428:MET:HG2	1:A:457:VAL:HG22	1.60	0.82
1:A:120:ASP:HA	1:A:262:ILE:O	1.80	0.81
1:A:247:ALA:N	1:A:255:ALA:O	2.13	0.81
1:A:199:ILE:HD13	1:A:200:ASP:H	1.44	0.80
1:A:236:LEU:CD2	1:A:262:ILE:HD12	2.12	0.80
1:A:500:LYS:CG	1:A:530:ALA:HB3	2.12	0.79
1:A:288:ILE:HG23	1:A:394:VAL:HG22	1.62	0.79
1:A:416:VAL:HG22	1:A:422:ILE:HG12	1.64	0.79
1:A:501:ILE:HD11	1:A:536:ILE:CD1	2.12	0.78
1:A:352:ASN:HB3	1:A:355:ARG:HD2	1.65	0.77
1:A:132:PRO:HD2	2:A:600:FAD:O5'	1.85	0.76
1:A:499:ARG:HG2	1:A:501:ILE:HD12	1.68	0.76
1:A:373:ASP:O	1:A:390:ARG:HD2	1.86	0.76
1:A:177:ALA:HA	3:A:705:HOH:O	1.85	0.75
1:A:500:LYS:HG2	1:A:530:ALA:HB3	1.66	0.75
1:A:561:ASP:O	1:A:564:ASP:HB2	1.86	0.75
1:A:508:TRP:CD1	1:A:523:PHE:HA	2.21	0.75
1:A:376:TYR:CE1	1:A:390:ARG:HG3	2.22	0.74
1:A:400:ARG:NH1	3:A:792:HOH:O	2.11	0.74
1:A:155:LYS:HD2	1:A:249:ASP:HA	1.67	0.73
1:A:529:ASP:HB3	1:A:532:THR:OG1	1.88	0.73
1:A:444:GLN:OE1	1:A:445:PRO:HA	1.89	0.73
1:A:123:TYR:O	1:A:265:PHE:HA	1.88	0.73
1:A:231:GLY:HA2	1:A:246:THR:HB	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:LYS:CE	1:A:522:PRO:HG3	2.18	0.72
1:A:535:ILE:HD12	1:A:535:ILE:N	2.03	0.72
1:A:305:LEU:HD22	1:A:306:ILE:H	1.54	0.72
1:A:444:GLN:OE1	1:A:446:MET:N	2.23	0.72
1:A:298:LYS:HE2	1:A:299:GLU:HG2	1.72	0.72
1:A:487:VAL:HG12	1:A:488:GLY:H	1.53	0.71
1:A:428:MET:HG2	1:A:457:VAL:CG2	2.21	0.71
1:A:589:THR:HG22	1:A:589:THR:O	1.92	0.70
1:A:535:ILE:HD12	1:A:535:ILE:H	1.55	0.70
1:A:295:LEU:CG	1:A:316:MET:HE1	2.21	0.69
1:A:207:ASP:OD2	3:A:716:HOH:O	2.11	0.68
1:A:489:GLU:HG2	1:A:501:ILE:CD1	2.23	0.68
1:A:127:VAL:HG11	1:A:138:ALA:HB2	1.75	0.68
1:A:473:VAL:HG22	1:A:487:VAL:HG12	1.76	0.68
1:A:444:GLN:OE1	1:A:444:GLN:HA	1.94	0.68
1:A:257:THR:HG22	1:A:259:GLU:HB2	1.75	0.68
1:A:501:ILE:CD1	1:A:536:ILE:HD11	2.20	0.68
1:A:162:LEU:O	1:A:162:LEU:HD12	1.94	0.67
1:A:157:LEU:HA	3:A:771:HOH:O	1.93	0.67
1:A:174:HIS:HD2	3:A:729:HOH:O	1.77	0.67
1:A:595:PRO:HB2	1:A:598:LYS:HD3	1.76	0.67
1:A:489:GLU:HB3	1:A:527:ILE:HD11	1.75	0.66
1:A:275:ARG:NH1	1:A:403:ASN:ND2	2.08	0.66
1:A:305:LEU:CD2	1:A:306:ILE:H	2.08	0.66
1:A:179:ILE:O	1:A:182:VAL:HG22	1.95	0.66
1:A:414:VAL:HA	1:A:431:ASN:HD21	1.59	0.66
1:A:350:LYS:HE3	1:A:350:LYS:HA	1.77	0.66
1:A:139:PHE:HE2	1:A:220:MET:HE3	1.60	0.65
1:A:499:ARG:HG2	1:A:501:ILE:CD1	2.26	0.65
1:A:186:ALA:O	1:A:189:GLY:N	2.27	0.65
1:A:206:LYS:HG2	1:A:207:ASP:N	2.11	0.65
1:A:527:ILE:HG13	1:A:527:ILE:O	1.89	0.65
1:A:336:LEU:O	1:A:337:MET:C	2.38	0.65
1:A:491:GLU:OE2	1:A:525:LYS:NZ	2.30	0.65
1:A:153:ARG:O	1:A:246:THR:HG21	1.97	0.65
1:A:199:ILE:HD13	1:A:199:ILE:C	2.21	0.64
1:A:276:VAL:HG13	3:A:714:HOH:O	1.96	0.64
1:A:303:LYS:HG2	1:A:326:ARG:CG	2.26	0.64
1:A:124:ASP:HB2	1:A:147:LYS:O	1.95	0.64
1:A:500:LYS:HG3	1:A:530:ALA:HB3	1.80	0.64
1:A:234:GLN:HG3	1:A:408:SER:OG	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ASP:OD1	3:A:762:HOH:O	2.15	0.64
1:A:154:TYR:CZ	1:A:252:GLU:HA	2.33	0.64
1:A:235:PHE:HB2	1:A:408:SER:O	1.97	0.63
1:A:305:LEU:HD22	1:A:306:ILE:N	2.13	0.63
1:A:494:ALA:O	1:A:498:ALA:N	2.32	0.62
1:A:236:LEU:HD22	1:A:262:ILE:HD12	1.82	0.62
1:A:358:ASN:HB2	1:A:360:MET:HE2	1.82	0.62
1:A:549:ILE:HD12	1:A:550:GLY:N	2.14	0.62
1:A:489:GLU:HG2	1:A:501:ILE:HD13	1.82	0.61
1:A:500:LYS:HG3	1:A:530:ALA:CB	2.30	0.61
1:A:529:ASP:O	1:A:533:GLY:N	2.31	0.61
1:A:519:CYS:O	1:A:522:PRO:CD	2.49	0.60
1:A:431:ASN:O	1:A:433:PRO:HD3	2.00	0.60
1:A:589:THR:O	1:A:589:THR:CG2	2.50	0.60
1:A:186:ALA:HA	1:A:190:ILE:O	2.02	0.60
1:A:164:VAL:HG11	1:A:252:GLU:OE1	2.01	0.60
1:A:363:THR:HG22	1:A:381:GLY:HA3	1.83	0.60
1:A:436:TYR:CE2	1:A:462:CYS:SG	2.94	0.59
1:A:453:HIS:HB3	1:A:469:PHE:CE1	2.26	0.59
1:A:544:ASN:O	1:A:547:ASP:N	2.35	0.59
1:A:305:LEU:HD21	1:A:330:VAL:HG22	1.84	0.59
1:A:499:ARG:CG	1:A:501:ILE:HD12	2.33	0.59
1:A:424:VAL:HG11	1:A:428:MET:HE3	1.84	0.59
1:A:427:GLN:O	1:A:428:MET:HB2	2.03	0.59
1:A:277:THR:HB	3:A:802:HOH:O	2.02	0.58
1:A:491:GLU:OE2	1:A:525:LYS:CE	2.51	0.58
1:A:436:TYR:HE2	1:A:462:CYS:HG	1.45	0.58
1:A:125:VAL:O	1:A:148:VAL:HA	2.03	0.58
1:A:436:TYR:HE2	1:A:462:CYS:SG	2.26	0.58
1:A:295:LEU:HG	1:A:316:MET:HE3	1.83	0.57
1:A:351:GLN:OE1	1:A:521:LYS:HD3	2.05	0.57
1:A:429:ARG:HG2	1:A:436:TYR:CE1	2.40	0.57
1:A:162:LEU:HD12	1:A:162:LEU:C	2.30	0.56
1:A:232:ASP:C	1:A:232:ASP:OD1	2.47	0.56
1:A:472:ARG:HG3	1:A:557:GLU:OE2	2.05	0.56
1:A:487:VAL:HG12	1:A:488:GLY:N	2.21	0.56
1:A:520:ASP:C	1:A:522:PRO:CD	2.78	0.56
1:A:152:GLU:OE1	2:A:600:FAD:H1B	2.06	0.56
1:A:321:SER:CB	1:A:355:ARG:HH11	2.15	0.56
1:A:367:ALA:HB3	1:A:378:THR:HB	1.88	0.56
1:A:343:ASP:OD1	1:A:525:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LEU:HD23	1:A:541:VAL:HG22	1.88	0.56
1:A:305:LEU:HD11	1:A:379:PHE:CE1	2.41	0.56
1:A:501:ILE:CG1	1:A:536:ILE:HD11	2.36	0.55
1:A:295:LEU:CD2	1:A:316:MET:HE1	2.35	0.55
1:A:440:ASP:OD1	2:A:600:FAD:H5'1	2.06	0.55
1:A:509:ALA:O	1:A:515:ILE:HD11	2.05	0.55
1:A:257:THR:CG2	1:A:259:GLU:HB2	2.36	0.55
1:A:544:ASN:N	3:A:799:HOH:O	2.39	0.55
1:A:572:HIS:HB2	1:A:577:GLU:OE1	2.07	0.55
1:A:494:ALA:HB2	1:A:501:ILE:HD13	1.88	0.55
1:A:551:GLU:HG2	1:A:579:ILE:HD13	1.88	0.55
1:A:341:ASP:HB3	1:A:343:ASP:OD1	2.06	0.55
1:A:336:LEU:HD23	1:A:348:TRP:HZ3	1.71	0.55
1:A:240:HIS:CD2	1:A:264:ALA:HB2	2.42	0.55
1:A:521:LYS:HG3	1:A:522:PRO:HD3	1.89	0.55
1:A:489:GLU:HG2	1:A:501:ILE:HD11	1.89	0.54
1:A:167:ILE:HD11	3:A:704:HOH:O	2.07	0.54
1:A:526:LEU:HD22	1:A:582:ALA:HB3	1.90	0.54
1:A:330:VAL:HG21	1:A:379:PHE:CE1	2.43	0.53
1:A:335:GLY:HA2	1:A:361:VAL:HG21	1.89	0.53
1:A:491:GLU:OE1	1:A:503:LYS:HE2	2.09	0.53
1:A:274:SER:HB2	1:A:401:ALA:O	2.08	0.53
1:A:146:LEU:HD13	1:A:146:LEU:N	2.24	0.53
1:A:173:LEU:HD21	1:A:315:GLU:HB3	1.90	0.53
1:A:342:ARG:HD2	1:A:492:LEU:HD21	1.91	0.52
1:A:291:SER:O	1:A:295:LEU:HD12	2.10	0.52
1:A:275:ARG:N	1:A:401:ALA:O	2.42	0.52
1:A:500:LYS:CG	1:A:530:ALA:CB	2.82	0.52
1:A:295:LEU:CG	1:A:316:MET:CE	2.79	0.52
1:A:520:ASP:C	1:A:522:PRO:HD3	2.30	0.52
1:A:398:ALA:HB3	3:A:802:HOH:O	2.10	0.52
1:A:141:ALA:O	1:A:144:GLU:HB2	2.09	0.51
1:A:486:TRP:CE3	1:A:486:TRP:N	2.77	0.51
1:A:508:TRP:HB2	1:A:522:PRO:HD2	1.92	0.51
1:A:367:ALA:HB3	1:A:378:THR:CB	2.41	0.51
1:A:440:ASP:OD2	1:A:446:MET:HB3	2.10	0.51
1:A:321:SER:HB2	1:A:327:LEU:HD11	1.91	0.51
1:A:254:ALA:HB2	3:A:811:HOH:O	2.10	0.51
1:A:174:HIS:CD2	3:A:729:HOH:O	2.57	0.51
1:A:275:ARG:HB3	1:A:403:ASN:HD21	1.75	0.51
1:A:521:LYS:NZ	1:A:522:PRO:HG3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:VAL:HG13	1:A:362:ASN:N	2.26	0.51
1:A:508:TRP:CB	1:A:522:PRO:O	2.56	0.50
1:A:459:ALA:O	1:A:462:CYS:HB2	2.11	0.50
1:A:351:GLN:OE1	1:A:521:LYS:HE3	2.11	0.50
1:A:364:LYS:HB2	1:A:380:GLU:HB3	1.94	0.50
1:A:414:VAL:HG21	1:A:435:ILE:HG21	1.94	0.50
1:A:155:LYS:HD2	1:A:249:ASP:CG	2.35	0.50
1:A:377:VAL:HG13	1:A:391:TYR:CE2	2.46	0.50
1:A:424:VAL:HG13	1:A:428:MET:HA	1.93	0.50
1:A:425:ASP:O	1:A:427:GLN:N	2.45	0.50
1:A:442:VAL:HG12	1:A:443:GLY:N	2.26	0.50
1:A:438:ILE:O	1:A:441:ILE:HG22	2.12	0.50
1:A:453:HIS:CB	1:A:469:PHE:HE1	2.14	0.50
1:A:293:GLY:O	1:A:294:ALA:C	2.52	0.50
1:A:161:CYS:HB2	2:A:600:FAD:O2'	2.11	0.49
1:A:395:LEU:HD12	1:A:396:VAL:N	2.27	0.49
1:A:561:ASP:H	1:A:564:ASP:HB2	1.76	0.49
1:A:305:LEU:HD11	1:A:379:PHE:CZ	2.47	0.49
1:A:344:LEU:HB3	1:A:484:VAL:HG13	1.94	0.49
1:A:405:LYS:HG3	1:A:416:VAL:HG11	1.93	0.49
1:A:440:ASP:CG	1:A:446:MET:HB3	2.37	0.49
1:A:230:GLN:CG	1:A:246:THR:CG2	2.72	0.49
1:A:421:PHE:CD2	1:A:443:GLY:HA2	2.48	0.49
1:A:563:ALA:HA	1:A:587:LEU:HD11	1.95	0.49
1:A:386:LYS:N	1:A:386:LYS:CD	2.57	0.48
1:A:293:GLY:O	1:A:296:ALA:N	2.34	0.48
1:A:508:TRP:CE3	1:A:522:PRO:HG2	2.48	0.48
2:A:600:FAD:N7A	3:A:790:HOH:O	2.35	0.48
1:A:350:LYS:HA	1:A:350:LYS:CE	2.39	0.48
1:A:544:ASN:O	1:A:545:GLY:C	2.57	0.48
1:A:517:ASN:N	1:A:517:ASN:HD22	2.12	0.48
1:A:519:CYS:C	1:A:522:PRO:HD3	2.39	0.48
1:A:236:LEU:HB3	1:A:240:HIS:HB2	1.96	0.48
1:A:358:ASN:CB	1:A:360:MET:HE2	2.44	0.48
1:A:237:ASP:O	1:A:239:HIS:N	2.47	0.47
1:A:328:ASP:HB3	1:A:360:MET:HE1	1.96	0.47
1:A:364:LYS:O	1:A:380:GLU:N	2.41	0.47
1:A:529:ASP:CG	1:A:532:THR:HG1	2.22	0.47
1:A:279:LEU:HB2	1:A:282:ILE:HD12	1.94	0.47
1:A:168:PRO:HB2	1:A:295:LEU:HD22	1.96	0.47
1:A:243:VAL:HG12	1:A:245:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ASP:OD1	1:A:427:GLN:HB2	2.14	0.47
1:A:489:GLU:O	1:A:537:GLY:HA3	2.13	0.47
1:A:251:TYR:O	1:A:252:GLU:HB2	2.14	0.47
1:A:551:GLU:OE2	1:A:570:HIS:NE2	2.38	0.47
1:A:127:VAL:CG1	1:A:138:ALA:HB2	2.44	0.47
1:A:131:GLY:O	1:A:135:TYR:HD2	1.97	0.47
1:A:211:SER:HA	1:A:214:THR:OG1	2.15	0.47
1:A:593:LEU:HB3	1:A:594:PRO:HD2	1.96	0.47
1:A:251:TYR:CD1	1:A:252:GLU:HG3	2.49	0.47
1:A:499:ARG:HG3	1:A:500:LYS:N	2.29	0.47
1:A:551:GLU:C	1:A:553:CYS:N	2.71	0.47
1:A:229:ILE:CG2	1:A:243:VAL:HG11	2.44	0.47
1:A:354:TYR:CD2	1:A:354:TYR:C	2.91	0.47
1:A:502:THR:HB	1:A:528:PHE:HB2	1.96	0.46
1:A:328:ASP:OD1	1:A:357:ASP:HB2	2.14	0.46
1:A:342:ARG:HD2	1:A:492:LEU:CD2	2.45	0.46
1:A:424:VAL:HG22	1:A:429:ARG:C	2.40	0.46
1:A:174:HIS:O	1:A:178:VAL:HG23	2.15	0.46
1:A:431:ASN:N	1:A:431:ASN:HD22	2.13	0.46
1:A:131:GLY:HA2	1:A:159:GLY:HA3	1.97	0.46
1:A:247:ALA:O	1:A:255:ALA:N	2.33	0.46
1:A:425:ASP:C	1:A:427:GLN:N	2.73	0.46
1:A:244:SER:HA	1:A:260:LYS:HG2	1.98	0.45
1:A:425:ASP:O	1:A:428:MET:N	2.39	0.45
1:A:549:ILE:HD12	1:A:549:ILE:C	2.41	0.45
1:A:349:GLN:HG2	3:A:773:HOH:O	2.17	0.45
1:A:424:VAL:CG1	1:A:428:MET:HE3	2.44	0.45
1:A:129:GLY:HA2	2:A:600:FAD:O4B	2.16	0.45
1:A:120:ASP:CA	1:A:262:ILE:O	2.58	0.45
1:A:429:ARG:HG2	1:A:436:TYR:HE1	1.79	0.45
1:A:312:ILE:HG23	3:A:784:HOH:O	2.16	0.45
1:A:301:PRO:HD2	1:A:320:TYR:CD1	2.51	0.45
1:A:365:THR:HG23	1:A:377:VAL:HG23	1.99	0.45
1:A:376:TYR:HA	1:A:389:GLN:O	2.17	0.45
1:A:165:GLY:O	1:A:166:CYS:C	2.61	0.44
1:A:167:ILE:CD1	3:A:704:HOH:O	2.64	0.44
1:A:336:LEU:N	1:A:336:LEU:CD1	2.80	0.44
1:A:206:LYS:O	1:A:207:ASP:C	2.60	0.44
1:A:544:ASN:CG	3:A:799:HOH:O	2.60	0.44
1:A:199:ILE:HG12	1:A:203:ARG:NH2	2.32	0.44
1:A:377:VAL:HG13	1:A:391:TYR:HE2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ILE:O	1:A:203:ARG:HB2	2.17	0.44
1:A:298:LYS:HE2	1:A:299:GLU:CG	2.45	0.44
1:A:501:ILE:CG1	1:A:527:ILE:HD12	2.41	0.44
1:A:554:LEU:O	1:A:558:MET:HG2	2.18	0.44
1:A:239:HIS:CE1	1:A:434:HIS:CD2	3.06	0.44
1:A:274:SER:CB	1:A:401:ALA:O	2.65	0.44
1:A:461:ASN:O	1:A:464:GLY:N	2.44	0.44
1:A:126:VAL:HG22	1:A:149:ALA:HB3	2.00	0.44
1:A:135:TYR:CD1	1:A:135:TYR:C	2.96	0.43
1:A:305:LEU:CD2	1:A:306:ILE:N	2.76	0.43
1:A:595:PRO:HG3	1:A:598:LYS:NZ	2.33	0.43
1:A:492:LEU:O	1:A:493:SER:C	2.60	0.43
1:A:565:ILE:O	1:A:568:THR:HB	2.19	0.43
1:A:124:ASP:O	1:A:266:LYS:HB2	2.19	0.43
1:A:157:LEU:HD11	1:A:228:VAL:HG21	2.00	0.43
1:A:352:ASN:O	1:A:353:GLU:C	2.62	0.43
1:A:351:GLN:OE1	1:A:482:PRO:HD3	2.19	0.43
1:A:501:ILE:HA	1:A:528:PHE:O	2.18	0.43
1:A:535:ILE:H	1:A:535:ILE:CD1	2.21	0.43
1:A:424:VAL:HG21	1:A:437:ALA:HB3	2.01	0.43
1:A:583:ALA:O	1:A:586:ALA:N	2.52	0.43
1:A:152:GLU:O	1:A:230:GLN:HA	2.19	0.43
1:A:274:SER:HA	1:A:402:PRO:HA	2.01	0.42
1:A:485:ALA:HB1	1:A:549:ILE:HG12	2.01	0.42
1:A:119:ALA:CB	1:A:261:LYS:HA	2.49	0.42
1:A:251:TYR:CE1	1:A:252:GLU:HG3	2.54	0.42
1:A:287:ARG:HH11	1:A:287:ARG:HD3	1.37	0.42
1:A:237:ASP:HB2	1:A:238:PRO:HD2	2.01	0.42
1:A:330:VAL:HG12	1:A:363:THR:OG1	2.19	0.42
1:A:173:LEU:HD13	1:A:319:VAL:CG1	2.48	0.42
1:A:282:ILE:HG21	1:A:288:ILE:HG21	2.00	0.42
1:A:425:ASP:C	1:A:427:GLN:H	2.26	0.42
1:A:527:ILE:HG12	1:A:537:GLY:HA3	2.01	0.42
1:A:146:LEU:HA	1:A:146:LEU:HD12	1.42	0.42
1:A:155:LYS:HD2	1:A:249:ASP:CA	2.44	0.42
1:A:346:LYS:HE2	1:A:346:LYS:HB2	1.92	0.42
1:A:119:ALA:HB1	1:A:261:LYS:HA	2.01	0.42
1:A:132:PRO:HG3	1:A:161:CYS:HB3	2.02	0.42
1:A:241:LEU:HD12	1:A:241:LEU:HA	1.68	0.42
1:A:551:GLU:C	1:A:553:CYS:H	2.27	0.42
1:A:583:ALA:O	1:A:586:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:GLY:O	1:A:135:TYR:CD2	2.73	0.42
1:A:353:GLU:CG	3:A:773:HOH:O	2.53	0.42
1:A:122:GLU:O	1:A:147:LYS:CE	2.68	0.41
1:A:275:ARG:NH1	1:A:275:ARG:HG2	2.35	0.41
1:A:274:SER:CA	1:A:401:ALA:O	2.67	0.41
1:A:382:ALA:O	1:A:383:ASN:C	2.62	0.41
1:A:549:ILE:HD12	1:A:550:GLY:H	1.82	0.41
1:A:199:ILE:C	1:A:199:ILE:CD1	2.84	0.41
1:A:489:GLU:CB	1:A:527:ILE:HD11	2.48	0.41
1:A:240:HIS:NE2	1:A:264:ALA:HB2	2.35	0.41
1:A:405:LYS:HE3	1:A:418:ASP:HA	2.03	0.41
1:A:519:CYS:O	1:A:522:PRO:CG	2.68	0.41
1:A:444:GLN:OE1	1:A:445:PRO:CA	2.65	0.41
1:A:522:PRO:HB2	1:A:541:VAL:O	2.20	0.41
1:A:123:TYR:CE2	1:A:149:ALA:HB2	2.55	0.41
1:A:155:LYS:HE2	1:A:155:LYS:HB2	1.46	0.41
1:A:309:GLY:O	1:A:314:LEU:HD11	2.20	0.41
1:A:414:VAL:CG2	1:A:435:ILE:HG21	2.51	0.41
1:A:584:GLU:O	1:A:585:VAL:C	2.64	0.41
1:A:572:HIS:HA	1:A:577:GLU:OE2	2.21	0.41
1:A:123:TYR:OH	1:A:227:ASP:OD2	2.31	0.41
1:A:213:LEU:HD23	1:A:213:LEU:HA	1.85	0.41
1:A:400:ARG:HD2	3:A:731:HOH:O	2.20	0.41
1:A:598:LYS:O	1:A:598:LYS:HD2	2.21	0.41
1:A:152:GLU:OE1	2:A:600:FAD:O2B	2.24	0.41
1:A:229:ILE:HD13	1:A:263:VAL:HG21	2.04	0.40
1:A:305:LEU:HD21	1:A:330:VAL:CG2	2.49	0.40
1:A:365:THR:HG23	1:A:377:VAL:CG2	2.50	0.40
1:A:535:ILE:HG12	1:A:565:ILE:HD11	2.03	0.40
1:A:370:PRO:HA	1:A:375:VAL:HA	2.02	0.40
1:A:427:GLN:OE1	1:A:429:ARG:NH2	2.55	0.40
1:A:514:ALA:HB1	1:A:519:CYS:O	2.20	0.40
1:A:522:PRO:CB	1:A:541:VAL:O	2.69	0.40
1:A:202:LEU:O	1:A:205:TYR:N	2.54	0.40
1:A:282:ILE:HG23	1:A:288:ILE:HD13	2.03	0.40
1:A:333:MET:HB2	1:A:338:GLN:CD	2.47	0.40
1:A:457:VAL:HG11	1:A:469:PHE:HA	2.02	0.40
1:A:257:THR:HG22	1:A:259:GLU:N	2.23	0.40
1:A:400:ARG:NH1	3:A:731:HOH:O	2.43	0.40
1:A:519:CYS:O	1:A:522:PRO:HG2	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ALA:CB	1:A:413:GLY:CA[4_565]	1.97	0.23
1:A:572:HIS:O	3:A:761:HOH:O[7_556]	2.00	0.20

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	480/482 (100%)	444 (92%)	30 (6%)	6 (1%)	9 18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	SER
1	A	185	LEU
1	A	238	PRO
1	A	426	LYS
1	A	285	ASP
1	A	337	MET

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	364/364 (100%)	277 (76%)	87 (24%)	1 1

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	ASP
1	A	125	VAL
1	A	127	VAL
1	A	146	LEU
1	A	147	LYS
1	A	155	LYS
1	A	164	VAL
1	A	167	ILE
1	A	170	LYS
1	A	172	LEU
1	A	173	LEU
1	A	179	ILE
1	A	181	GLU
1	A	199	ILE
1	A	205	TYR
1	A	206	LYS
1	A	212	ARG
1	A	223	SER
1	A	225	LYS
1	A	232	ASP
1	A	236	LEU
1	A	241	LEU
1	A	246	THR
1	A	249	ASP
1	A	253	GLN
1	A	259	GLU
1	A	266	LYS
1	A	276	VAL
1	A	284	GLU
1	A	305	LEU
1	A	319	VAL
1	A	321	SER
1	A	325	SER
1	A	326	ARG
1	A	327	LEU
1	A	329	VAL
1	A	330	VAL
1	A	334	ASP
1	A	336	LEU
1	A	338	GLN
1	A	342	ARG
1	A	344	LEU
1	A	346	LYS

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Mol	Chain	Res	Type
1	A	350	LYS
1	A	361	VAL
1	A	364	LYS
1	A	366	VAL
1	A	377	VAL
1	A	386	LYS
1	A	394	VAL
1	A	396	VAL
1	A	408	SER
1	A	411	LYS
1	A	419	ARG
1	A	423	GLU
1	A	424	VAL
1	A	426	LYS
1	A	428	MET
1	A	429	ARG
1	A	431	ASN
1	A	433	PRO
1	A	442	VAL
1	A	457	VAL
1	A	466	LYS
1	A	473	VAL
1	A	481	SER
1	A	486	TRP
1	A	487	VAL
1	A	492	LEU
1	A	495	LYS
1	A	499	ARG
1	A	500	LYS
1	A	501	ILE
1	A	503	LYS
1	A	517	ASN
1	A	521	LYS
1	A	525	LYS
1	A	526	LEU
1	A	527	ILE
1	A	534	ARG
1	A	535	ILE
1	A	541	VAL
1	A	549	ILE
1	A	552	VAL
1	A	553	CYS

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Mol	Chain	Res	Type
1	A	581	MET
1	A	598	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	GLN
1	A	403	ASN
1	A	431	ASN
1	A	517	ASN

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAD	A	600	-	58,58,58	2.00	18 (31%)	85,89,89	2.38	36 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	600	-	3/3/9/9	13/34/50/50	0/6/6/6

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C1'-C2'	4.92	1.59	1.52
2	A	600	FAD	C4X-N5	4.32	1.40	1.30
2	A	600	FAD	C1'-N10	-4.06	1.38	1.47
2	A	600	FAD	C6-C5X	3.92	1.45	1.40
2	A	600	FAD	C9-C9A	3.91	1.46	1.39
2	A	600	FAD	C10-N10	3.60	1.45	1.37
2	A	600	FAD	C5'-C4'	-3.48	1.47	1.51
2	A	600	FAD	PA-O2A	-3.05	1.41	1.55
2	A	600	FAD	C10-N1	3.02	1.39	1.33
2	A	600	FAD	C5B-C4B	2.87	1.60	1.51
2	A	600	FAD	O2B-C2B	2.63	1.49	1.43
2	A	600	FAD	C2'-C3'	2.61	1.58	1.53
2	A	600	FAD	C2A-N3A	2.51	1.38	1.33
2	A	600	FAD	C9A-C5X	-2.49	1.37	1.41
2	A	600	FAD	P-O3P	-2.21	1.57	1.59
2	A	600	FAD	P-O1P	-2.21	1.43	1.50
2	A	600	FAD	C2B-C3B	-2.17	1.47	1.53
2	A	600	FAD	C4A-N3A	2.01	1.38	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	O3P-PA-O1A	5.44	127.05	110.70
2	A	600	FAD	C4-N3-C2	-5.42	116.02	125.64
2	A	600	FAD	O5'-P-O1P	-5.11	88.68	108.94
2	A	600	FAD	O2P-P-O1P	-5.07	88.87	112.44
2	A	600	FAD	O2A-PA-O1A	-4.97	89.33	112.44
2	A	600	FAD	C4-C4X-N5	4.82	124.86	118.21
2	A	600	FAD	C5X-C9A-N10	4.57	122.10	117.97
2	A	600	FAD	C2B-C1B-N9A	-4.02	103.32	113.30
2	A	600	FAD	O4-C4-N3	-3.85	112.87	120.11
2	A	600	FAD	C9A-N10-C10	-3.70	115.11	120.75
2	A	600	FAD	C7M-C7-C6	-3.68	113.09	119.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	O3B-C3B-C4B	-3.65	100.61	111.08
2	A	600	FAD	C4X-C4-N3	3.42	121.97	113.25
2	A	600	FAD	C1'-N10-C9A	3.40	127.23	120.63
2	A	600	FAD	O2P-P-O5'	3.38	122.91	107.57
2	A	600	FAD	O2B-C2B-C1B	-3.33	98.63	110.10
2	A	600	FAD	O2A-PA-O3P	-3.12	98.85	107.27
2	A	600	FAD	N10-C10-N1	-3.11	109.36	118.51
2	A	600	FAD	N3-C2-N1	2.99	125.86	119.50
2	A	600	FAD	C10-C4X-N5	-2.93	118.82	124.81
2	A	600	FAD	O4B-C4B-C3B	2.91	110.92	105.15
2	A	600	FAD	C7M-C7-C8	2.85	126.58	120.76
2	A	600	FAD	C4X-C10-N1	-2.62	118.16	124.59
2	A	600	FAD	C9-C9A-C5X	-2.44	115.72	120.03
2	A	600	FAD	C5'-C4'-C3'	-2.39	107.71	112.22
2	A	600	FAD	C4A-N9A-C1B	-2.30	121.24	126.63
2	A	600	FAD	O2-C2-N1	-2.30	117.98	121.80
2	A	600	FAD	O4B-C4B-C5B	2.21	116.42	109.33
2	A	600	FAD	O5B-C5B-C4B	-2.15	101.66	108.99
2	A	600	FAD	O5B-PA-O1A	2.15	117.45	108.94
2	A	600	FAD	O2'-C2'-C3'	-2.10	104.33	109.25
2	A	600	FAD	C5B-C4B-C3B	-2.09	107.68	115.21
2	A	600	FAD	C9A-C9-C8	2.07	123.39	119.22
2	A	600	FAD	C2'-C1'-N10	2.03	119.81	110.20
2	A	600	FAD	C4A-N9A-C8A	2.01	107.84	105.74
2	A	600	FAD	C6-C5X-C9A	2.00	121.80	119.05

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	600	FAD	C2'
2	A	600	FAD	C4'
2	A	600	FAD	C3'

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	N10-C1'-C2'-O2'
2	A	600	FAD	N10-C1'-C2'-C3'
2	A	600	FAD	O4'-C4'-C5'-O5'
2	A	600	FAD	PA-O3P-P-O5'
2	A	600	FAD	O4B-C4B-C5B-O5B
2	A	600	FAD	C2'-C1'-N10-C9A

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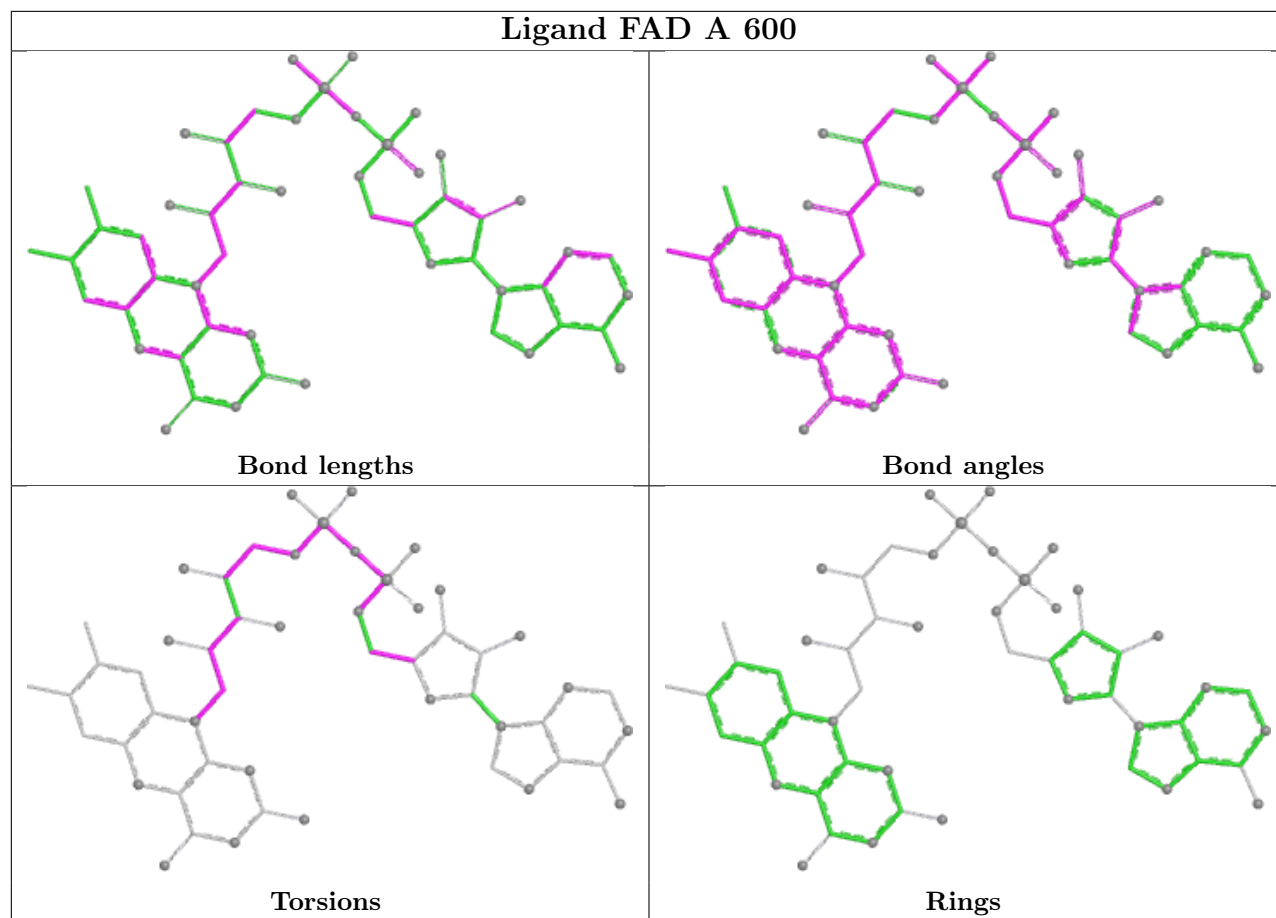
Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C5B-O5B-PA-O1A
2	A	600	FAD	C5'-O5'-P-O1P
2	A	600	FAD	C5'-O5'-P-O3P
2	A	600	FAD	C4'-C5'-O5'-P
2	A	600	FAD	C3'-C4'-C5'-O5'
2	A	600	FAD	O2'-C2'-C3'-C4'
2	A	600	FAD	P-O3P-PA-O2A

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	7	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.