



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:51 AM UTC

PDB ID : 6EM0 / pdb_00006em0
Title : Crystal Structure of 2-hydroxybiphenyl 3-monooxygenase M321A from *Pseudomonas azelaica*
Authors : Deri, B.; Bregman-Cohen, A.; Pazy Benhar, Y.; Fishman, A.
Deposited on : 2017-10-01
Resolution : 2.78 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	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

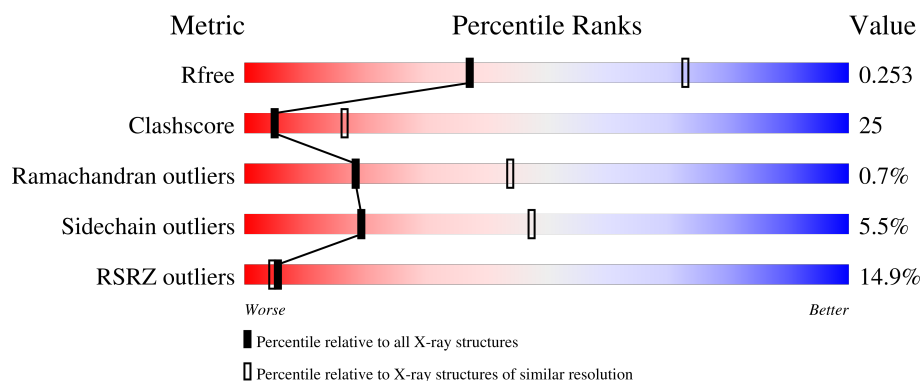
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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))
R_{free}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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 $\leq 5\%$. 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	581	14% 56% 32% 7% • •
1	B	581	15% 54% 33% 9% • •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8963 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.

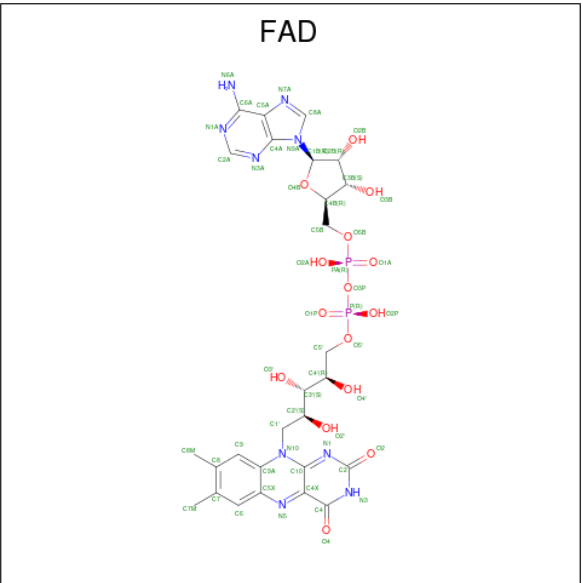
- Molecule 1 is a protein called 2-hydroxybiphenyl-3-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	566	Total	C	N	O	S	0	0	0
			4344	2744	764	817	19			
1	B	565	Total	C	N	O	S	0	0	0
			4337	2739	763	816	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	321	ALA	MET	engineered mutation	UNP O06647
B	321	ALA	MET	engineered mutation	UNP O06647

- 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		

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

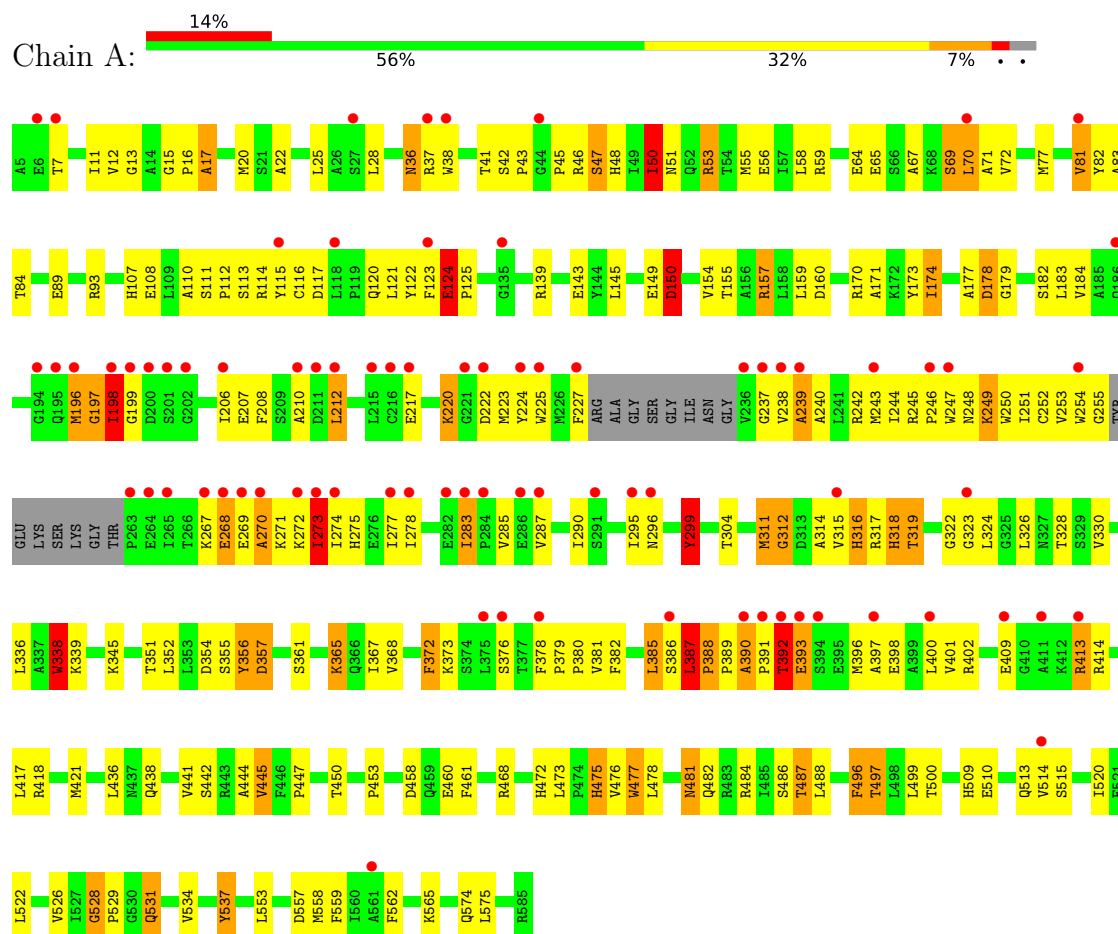
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total	O	0	0
			102	102		
3	B	74	Total	O	0	0
			74	74		

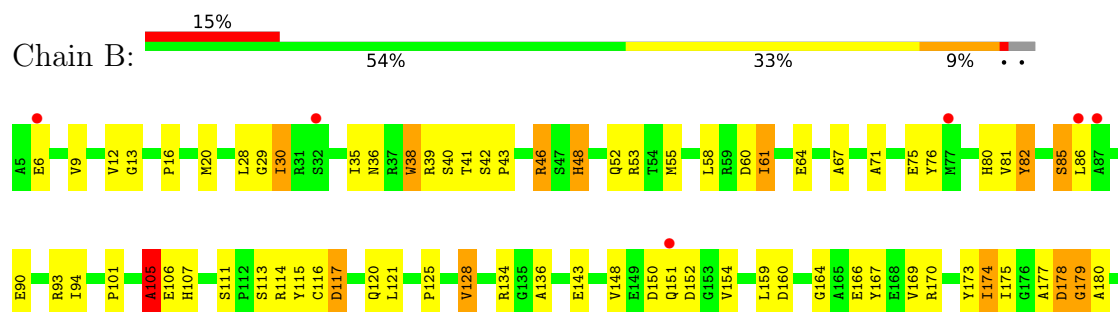
3 Residue-property plots

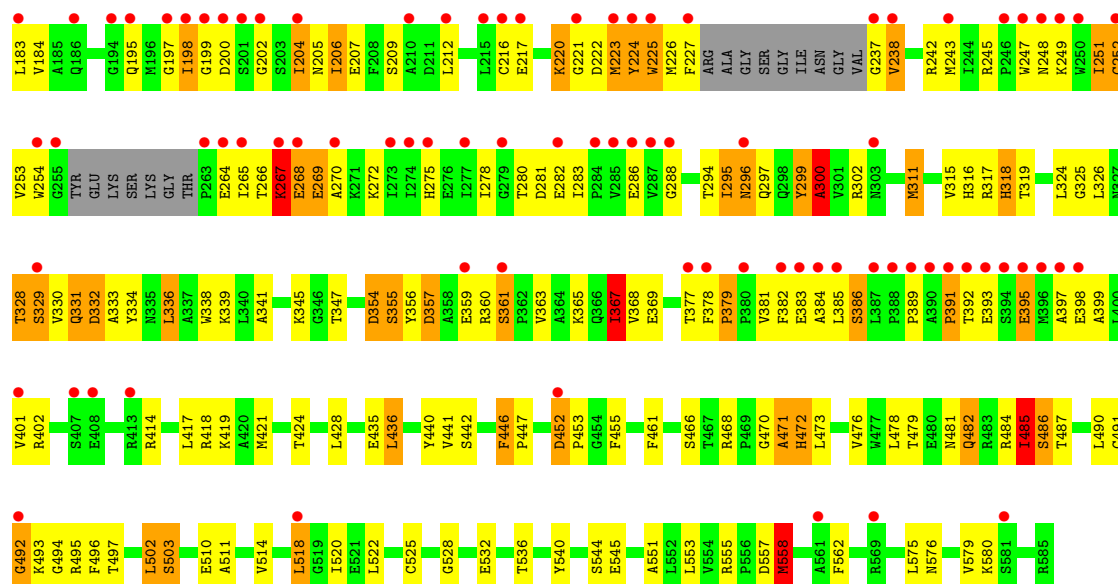
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 2-hydroxybiphenyl-3-monooxygenase



• Molecule 1: 2-hydroxybiphenyl-3-monooxygenase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.57Å 130.96Å 79.08Å 90.00° 98.96° 90.00°	Depositor
Resolution (Å)	50.18 – 2.78 50.18 – 2.78	Depositor EDS
% Data completeness (in resolution range)	88.6 (50.18-2.78) 88.6 (50.18-2.78)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.226 , 0.253 0.233 , 0.253	Depositor DCC
R_{free} test set	1716 reflections (4.38%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8963	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.91% 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	2.21	77/4439 (1.7%)	1.63	106/6017 (1.8%)
1	B	2.48	86/4432 (1.9%)	1.74	113/6007 (1.9%)
All	All	2.35	163/8871 (1.8%)	1.69	219/12024 (1.8%)

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	1	4
1	B	0	8
All	All	1	12

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	ILE	C-N	37.92	1.66	1.33
1	B	472	HIS	N-CA	36.39	1.91	1.46
1	A	528	GLY	C-O	-35.10	0.76	1.24
1	B	446	PHE	C-O	-35.09	0.81	1.24
1	B	355	SER	N-CA	33.35	1.91	1.46
1	B	82	TYR	C-N	-32.03	0.93	1.33
1	A	47	SER	C-O	-30.67	0.81	1.23
1	B	296	ASN	C-O	-30.06	0.88	1.24
1	B	101	PRO	CA-CB	-29.66	1.11	1.53
1	A	528	GLY	CA-C	28.66	1.92	1.51
1	B	471	ALA	C-N	-28.50	0.93	1.33
1	B	179	GLY	C-N	27.45	1.70	1.34
1	B	128	VAL	CA-CB	26.83	1.88	1.54
1	B	354	ASP	C-N	-26.80	0.96	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	296	ASN	CA-C	26.12	1.86	1.52
1	A	69	SER	C-N	25.45	1.67	1.33
1	B	502	LEU	CA-C	25.19	1.85	1.52
1	B	502	LEU	C-N	-25.08	0.99	1.33
1	A	50	ILE	CA-CB	24.96	1.84	1.53
1	B	300	ALA	N-CA	23.88	1.76	1.46
1	B	331	GLN	CA-CB	23.75	1.92	1.53
1	B	347	THR	CB-OG1	-23.07	1.06	1.43
1	A	69	SER	C-O	-22.52	0.94	1.24
1	B	105	ALA	CA-C	20.70	1.81	1.52
1	B	30	ILE	CA-C	-20.02	1.30	1.53
1	A	299	TYR	C-O	19.77	1.49	1.23
1	B	30	ILE	N-CA	19.32	1.67	1.46
1	A	47	SER	CA-C	18.80	1.78	1.53
1	B	105	ALA	C-N	-17.21	1.07	1.33
1	A	531	GLN	CA-CB	16.47	1.77	1.53
1	B	518	LEU	CA-CB	16.27	1.80	1.53
1	A	50	ILE	CB-CG1	15.90	1.85	1.53
1	B	179	GLY	CA-C	-15.84	1.31	1.51
1	A	372	PHE	CE1-CZ	15.48	1.85	1.38
1	B	300	ALA	CA-C	-15.10	1.31	1.52
1	A	528	GLY	C-N	14.95	1.51	1.33
1	A	47	SER	C-N	14.61	1.54	1.33
1	B	389	PRO	N-CD	-14.43	1.27	1.47
1	B	300	ALA	CA-CB	-14.02	1.31	1.53
1	A	497	THR	CA-CB	-13.62	1.33	1.53
1	A	239	ALA	C-O	12.97	1.38	1.23
1	B	395	GLU	C-O	-12.96	1.06	1.24
1	A	497	THR	N-CA	-12.88	1.30	1.46
1	A	477	TRP	C-N	-12.72	1.17	1.33
1	A	50	ILE	CB-CG2	-12.61	1.10	1.52
1	A	150	ASP	C-N	-12.61	1.16	1.33
1	A	513	GLN	CG-CD	-12.35	1.21	1.52
1	B	30	ILE	CA-CB	-12.22	1.39	1.53
1	A	69	SER	CA-C	11.97	1.69	1.52
1	A	531	GLN	CB-CG	11.84	1.88	1.52
1	B	332	ASP	CG-OD1	11.77	1.47	1.25
1	A	149	GLU	CB-CG	-11.65	1.17	1.52
1	A	338	TRP	C-O	-10.84	1.10	1.24
1	A	299	TYR	C-N	-10.68	1.18	1.33
1	A	299	TYR	CA-C	-10.14	1.40	1.52
1	A	268	GLU	CB-CG	9.99	1.82	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	331	GLN	CB-CG	9.29	1.80	1.52
1	A	318	HIS	C-O	-8.88	1.15	1.24
1	B	328	THR	C-N	-8.40	1.23	1.33
1	A	413	ARG	C-N	8.39	1.45	1.33
1	B	61	ILE	CB-CG1	-8.34	1.36	1.53
1	B	48	HIS	C-O	-8.27	1.14	1.23
1	A	198	ILE	CA-C	-8.12	1.42	1.52
1	B	296	ASN	C-N	8.06	1.45	1.33
1	A	198	ILE	C-O	-8.01	1.14	1.24
1	A	381	VAL	C-N	-7.64	1.23	1.33
1	A	414	ARG	C-N	7.63	1.44	1.33
1	B	93	ARG	C-N	-7.54	1.25	1.33
1	A	497	THR	CA-C	7.51	1.61	1.52
1	B	485	ILE	C-O	-7.20	1.17	1.24
1	B	175	ILE	C-O	-6.99	1.16	1.24
1	B	81	VAL	C-N	-6.98	1.23	1.33
1	A	319	THR	CB-OG1	-6.84	1.32	1.43
1	B	12	VAL	C-O	-6.81	1.15	1.23
1	B	9	VAL	C-O	-6.73	1.17	1.24
1	B	128	VAL	CB-CG2	-6.72	1.30	1.52
1	B	357	ASP	C-O	-6.69	1.16	1.24
1	B	116	CYS	C-N	6.66	1.44	1.33
1	A	124	GLU	N-CA	-6.63	1.41	1.46
1	B	224	TYR	C-O	-6.61	1.16	1.23
1	B	576	ASN	CA-CB	6.45	1.63	1.53
1	A	357	ASP	C-O	-6.27	1.16	1.24
1	B	311	MET	C-O	-6.26	1.17	1.23
1	B	105	ALA	C-O	6.17	1.32	1.24
1	A	125	PRO	C-O	-6.13	1.16	1.24
1	B	179	GLY	C-O	-6.10	1.15	1.24
1	A	51	ASN	C-O	-6.10	1.15	1.23
1	A	499	LEU	C-O	-6.10	1.16	1.24
1	B	61	ILE	CG1-CD1	-6.06	1.28	1.51
1	A	559	PHE	C-O	-6.05	1.16	1.23
1	B	93	ARG	C-O	-6.02	1.16	1.23
1	A	497	THR	C-O	-5.98	1.17	1.24
1	A	224	TYR	C-O	-5.92	1.17	1.24
1	A	372	PHE	CD1-CE1	-5.90	1.21	1.38
1	B	486	SER	C-O	-5.84	1.16	1.23
1	B	206	ILE	C-O	-5.83	1.17	1.24
1	A	11	ILE	C-O	-5.82	1.18	1.24
1	B	253	VAL	C-O	-5.81	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	466	SER	C-O	-5.81	1.16	1.23
1	A	65	GLU	C-O	-5.80	1.17	1.24
1	B	468	ARG	CA-C	-5.79	1.46	1.53
1	B	367	ILE	C-O	-5.78	1.17	1.24
1	A	368	VAL	C-N	-5.74	1.25	1.33
1	B	38	TRP	C-O	5.65	1.31	1.23
1	A	500	THR	C-O	-5.64	1.17	1.23
1	B	319	THR	C-N	5.64	1.38	1.33
1	A	444	ALA	C-O	-5.62	1.16	1.24
1	B	81	VAL	C-O	-5.62	1.17	1.24
1	A	53	ARG	C-O	-5.60	1.17	1.24
1	B	316	HIS	C-O	-5.58	1.17	1.24
1	A	253	VAL	C-N	5.57	1.40	1.33
1	A	36	ASN	C-O	-5.55	1.17	1.23
1	A	365	LYS	C-O	-5.54	1.17	1.24
1	B	82	TYR	C-O	-5.54	1.17	1.24
1	A	312	GLY	C-O	-5.53	1.15	1.23
1	B	315	VAL	C-O	-5.52	1.18	1.24
1	B	540	TYR	C-O	-5.52	1.17	1.24
1	A	526	VAL	C-O	-5.51	1.18	1.24
1	B	173	TYR	C-O	-5.51	1.17	1.23
1	A	110	ALA	C-O	-5.49	1.16	1.24
1	A	316	HIS	C-O	-5.48	1.17	1.24
1	A	368	VAL	C-O	-5.48	1.17	1.24
1	B	143	GLU	C-O	-5.45	1.17	1.24
1	B	368	VAL	C-O	-5.43	1.17	1.24
1	B	148	VAL	C-O	-5.43	1.18	1.24
1	B	174	ILE	C-O	-5.43	1.18	1.24
1	B	525	CYS	C-O	-5.42	1.17	1.24
1	B	107	HIS	C-O	-5.39	1.17	1.24
1	B	326	LEU	C-O	-5.37	1.17	1.24
1	A	116	CYS	CA-C	-5.36	1.46	1.52
1	A	174	ILE	C-O	-5.35	1.18	1.24
1	A	458	ASP	C-O	-5.34	1.17	1.24
1	B	117	ASP	C-O	-5.33	1.17	1.24
1	B	136	ALA	C-O	-5.33	1.17	1.23
1	B	329	SER	C-N	5.32	1.40	1.33
1	B	125	PRO	C-O	-5.31	1.17	1.24
1	A	58	LEU	C-O	-5.30	1.17	1.24
1	B	476	VAL	C-O	-5.29	1.17	1.23
1	B	455	PHE	N-CA	-5.27	1.39	1.46
1	B	558	MET	C-O	-5.26	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	502	LEU	C-O	5.26	1.30	1.24
1	B	470	GLY	C-O	-5.26	1.16	1.24
1	B	35	ILE	C-O	-5.25	1.17	1.23
1	A	476	VAL	C-O	-5.21	1.16	1.23
1	A	250	TRP	C-O	-5.21	1.17	1.24
1	B	496	PHE	N-CA	5.20	1.52	1.45
1	B	497	THR	C-O	-5.20	1.17	1.23
1	A	22	ALA	C-O	-5.19	1.17	1.24
1	A	116	CYS	N-CA	-5.18	1.39	1.45
1	A	67	ALA	C-O	-5.16	1.18	1.24
1	A	12	VAL	CA-C	-5.16	1.47	1.52
1	B	551	ALA	C-O	-5.11	1.17	1.23
1	B	532	GLU	C-O	-5.10	1.18	1.24
1	A	157	ARG	C-O	-5.09	1.17	1.24
1	A	17	ALA	C-O	-5.08	1.18	1.24
1	B	318	HIS	C-O	-5.08	1.17	1.24
1	A	367	ILE	C-O	-5.08	1.17	1.24
1	A	160	ASP	C-O	-5.06	1.18	1.24
1	A	445	VAL	C-O	-5.03	1.18	1.24
1	A	139	ARG	C-O	-5.02	1.17	1.24
1	A	25	LEU	C-O	-5.01	1.18	1.24
1	A	173	TYR	C-O	-5.01	1.17	1.23
1	B	94	ILE	C-O	-5.00	1.19	1.24

All (219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	528	GLY	O-C-N	28.49	150.26	121.77
1	B	502	LEU	O-C-N	27.88	151.67	122.12
1	B	300	ALA	CB-CA-C	26.19	146.46	110.06
1	B	502	LEU	CA-C-O	-24.55	94.52	120.55
1	B	30	ILE	CB-CA-C	22.69	135.73	111.23
1	B	296	ASN	O-C-N	22.06	149.31	123.05
1	B	446	PHE	O-C-N	20.16	139.34	121.20
1	B	179	GLY	O-C-N	-19.36	103.50	122.86
1	B	105	ALA	CA-C-O	-19.03	94.75	119.11
1	B	179	GLY	CA-C-O	17.90	150.46	122.71
1	B	61	ILE	CB-CG1-CD1	17.16	149.83	113.80
1	B	354	ASP	O-C-N	16.89	143.05	122.27
1	A	497	THR	N-CA-CB	15.59	134.97	110.65
1	A	528	GLY	CA-C-N	-15.52	103.07	119.83
1	A	528	GLY	C-N-CA	-15.52	103.07	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	GLU	CB-CG-CD	15.26	138.54	112.60
1	B	446	PHE	CA-C-O	-14.79	104.90	119.24
1	A	198	ILE	CA-C-O	14.72	139.17	120.78
1	A	47	SER	O-C-N	14.37	139.56	122.75
1	A	50	ILE	CA-CB-CG1	-14.32	86.05	110.40
1	A	477	TRP	O-C-N	-14.21	106.76	123.10
1	A	299	TYR	CA-C-O	-14.18	104.95	121.68
1	A	338	TRP	CA-C-O	-13.80	104.51	120.10
1	A	198	ILE	O-C-N	-13.66	105.49	122.57
1	A	372	PHE	CG-CD1-CE1	12.97	142.76	120.70
1	B	576	ASN	CA-CB-CG	-12.93	99.67	112.60
1	B	492	GLY	N-CA-C	12.83	139.82	114.16
1	A	531	GLN	CA-CB-CG	-12.58	88.94	114.10
1	B	331	GLN	CA-CB-CG	-12.49	89.12	114.10
1	B	332	ASP	CA-CB-CG	12.39	124.99	112.60
1	A	372	PHE	CD1-CE1-CZ	-12.21	98.03	120.00
1	A	497	THR	CA-C-O	-12.10	107.35	120.30
1	A	41	THR	N-CA-C	-11.99	92.72	110.46
1	A	299	TYR	O-C-N	-11.95	105.85	122.94
1	B	128	VAL	CA-CB-CG1	-11.40	91.03	110.40
1	A	150	ASP	O-C-N	-11.36	110.03	123.10
1	B	471	ALA	O-C-N	11.35	138.74	122.97
1	B	296	ASN	CA-C-N	-11.27	105.01	121.24
1	B	296	ASN	C-N-CA	-11.27	105.01	121.24
1	A	69	SER	N-CA-C	11.06	126.88	113.16
1	A	338	TRP	O-C-N	11.06	135.16	122.22
1	B	61	ILE	CA-CB-CG1	10.97	129.05	110.40
1	B	41	THR	N-CA-C	-10.91	96.45	110.53
1	A	477	TRP	CA-C-N	10.66	139.35	121.87
1	A	477	TRP	C-N-CA	10.66	139.35	121.87
1	A	537	TYR	CB-CG-CD1	10.54	136.61	120.80
1	A	537	TYR	CB-CG-CD2	-10.38	105.23	120.80
1	A	50	ILE	N-CA-CB	10.28	124.62	111.67
1	A	239	ALA	O-C-N	-10.05	109.33	121.79
1	B	268	GLU	N-CA-C	-9.95	98.17	113.89
1	A	268	GLU	N-CA-CB	9.89	127.98	110.18
1	A	478	LEU	N-CA-CB	9.30	126.26	111.56
1	B	81	VAL	N-CA-C	9.20	121.52	108.36
1	A	47	SER	N-CA-C	-9.17	98.42	110.43
1	B	101	PRO	CA-CB-CG	8.94	121.48	104.50
1	B	42	SER	N-CA-C	8.87	122.26	109.48
1	A	239	ALA	CA-C-O	8.85	131.98	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	389	PRO	CA-N-CD	8.84	124.38	112.00
1	A	513	GLN	CA-CB-CG	-8.74	96.62	114.10
1	B	178	ASP	N-CA-C	8.69	123.61	112.92
1	A	69	SER	CA-C-O	8.69	129.79	119.28
1	A	268	GLU	CA-CB-CG	-8.68	96.74	114.10
1	A	413	ARG	CA-C-N	-8.67	108.67	120.28
1	A	413	ARG	C-N-CA	-8.67	108.67	120.28
1	B	30	ILE	CA-CB-CG1	8.51	124.86	110.40
1	A	392	THR	OG1-CB-CG2	8.41	126.12	109.30
1	A	50	ILE	CB-CA-C	-8.39	99.53	111.19
1	B	300	ALA	CA-C-O	-8.14	112.01	120.80
1	A	38	TRP	N-CA-C	8.12	121.00	110.53
1	A	319	THR	OG1-CB-CG2	8.07	125.44	109.30
1	A	497	THR	CA-CB-CG2	7.99	124.08	110.50
1	A	393	GLU	N-CA-C	7.91	121.44	111.24
1	B	332	ASP	OD1-CG-OD2	-7.88	103.99	122.90
1	A	268	GLU	CB-CG-CD	7.85	125.94	112.60
1	A	69	SER	CB-CA-C	-7.80	95.97	110.01
1	A	299	TYR	CA-C-N	7.71	133.36	122.72
1	A	299	TYR	C-N-CA	7.71	133.36	122.72
1	A	513	GLN	CG-CD-NE2	7.67	127.90	116.40
1	B	38	TRP	N-CA-C	7.65	122.21	110.36
1	A	237	GLY	CA-C-N	-7.59	114.25	122.59
1	A	237	GLY	C-N-CA	-7.59	114.25	122.59
1	B	576	ASN	CB-CG-ND2	-7.53	105.11	116.40
1	B	30	ILE	CA-C-O	-7.44	111.61	120.76
1	B	436	LEU	N-CA-C	7.44	123.91	114.31
1	A	47	SER	CA-C-N	-7.34	107.53	121.54
1	A	47	SER	C-N-CA	-7.34	107.53	121.54
1	A	531	GLN	CB-CA-C	-7.24	97.12	111.60
1	B	85	SER	N-CA-C	-7.12	96.75	108.07
1	B	29	GLY	CA-C-N	7.08	132.07	122.01
1	B	29	GLY	C-N-CA	7.08	132.07	122.01
1	A	197	GLY	N-CA-C	-7.07	96.43	113.18
1	B	356	TYR	N-CA-C	-6.97	103.77	111.36
1	A	385	LEU	N-CA-C	-6.93	104.82	112.72
1	B	518	LEU	N-CA-CB	6.88	120.61	110.56
1	B	331	GLN	CB-CG-CD	-6.88	100.91	112.60
1	B	81	VAL	CB-CA-C	-6.86	101.51	110.84
1	B	52	GLN	N-CA-C	6.82	119.55	111.71
1	A	392	THR	N-CA-C	-6.79	99.51	109.63
1	B	354	ASP	CA-C-N	-6.79	107.74	121.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	354	ASP	C-N-CA	-6.79	107.74	121.18
1	A	387	LEU	CA-C-N	6.77	127.36	120.38
1	A	387	LEU	C-N-CA	6.77	127.36	120.38
1	B	205	ASN	N-CA-C	6.75	119.42	108.41
1	B	225	TRP	N-CA-C	6.73	120.63	109.46
1	A	178	ASP	N-CA-C	6.72	120.38	112.72
1	A	81	VAL	N-CA-C	6.69	117.76	107.99
1	B	81	VAL	CA-C-N	6.64	131.89	122.72
1	B	81	VAL	C-N-CA	6.64	131.89	122.72
1	A	513	GLN	CB-CG-CD	6.58	123.79	112.60
1	B	105	ALA	CB-CA-C	-6.58	96.87	109.95
1	B	38	TRP	CA-C-O	-6.57	113.87	121.82
1	B	105	ALA	O-C-N	6.52	131.95	122.43
1	A	461	PHE	N-CA-C	6.48	119.67	111.69
1	A	478	LEU	N-CA-C	-6.38	99.46	108.96
1	B	299	TYR	CA-C-N	6.34	131.34	121.26
1	B	299	TYR	C-N-CA	6.34	131.34	121.26
1	A	436	LEU	N-CA-C	6.33	121.95	113.72
1	A	513	GLN	CG-CD-OE1	-6.33	108.14	120.80
1	B	179	GLY	N-CA-C	-6.32	101.34	112.77
1	A	253	VAL	O-C-N	6.30	130.04	123.05
1	A	149	GLU	CG-CD-OE1	-6.25	104.04	118.40
1	B	379	PRO	CA-C-N	-6.24	113.71	119.82
1	B	379	PRO	C-N-CA	-6.24	113.71	119.82
1	A	460	GLU	N-CA-C	-6.22	105.34	113.12
1	A	318	HIS	N-CA-C	6.22	116.06	107.73
1	A	453	PRO	N-CA-C	6.22	121.63	113.86
1	B	399	ALA	N-CA-C	-6.22	97.56	110.80
1	A	496	PHE	CA-C-N	6.17	131.71	123.00
1	A	496	PHE	C-N-CA	6.17	131.71	123.00
1	A	69	SER	CA-C-N	-6.15	112.90	122.37
1	A	69	SER	C-N-CA	-6.15	112.90	122.37
1	B	128	VAL	CA-CB-CG2	-6.13	99.97	110.40
1	A	84	THR	N-CA-C	-6.09	103.98	112.45
1	A	198	ILE	N-CA-C	-6.08	96.69	109.34
1	A	155	THR	N-CA-C	-6.07	99.11	109.24
1	A	481	ASN	N-CA-C	-6.04	104.03	112.25
1	B	389	PRO	N-CA-CB	-6.02	96.93	103.25
1	A	83	ALA	N-CA-C	6.00	116.20	108.34
1	A	268	GLU	CB-CA-C	-5.99	96.76	110.18
1	A	304	THR	N-CA-C	5.97	118.63	108.90
1	B	347	THR	CA-CB-OG1	-5.88	100.79	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	SER	CB-CA-C	5.87	120.12	110.03
1	B	116	CYS	CA-C-N	-5.86	114.79	123.11
1	B	116	CYS	C-N-CA	-5.86	114.79	123.11
1	B	164	GLY	N-CA-C	-5.85	108.12	115.08
1	A	319	THR	CA-CB-OG1	-5.82	100.87	109.60
1	A	179	GLY	N-CA-C	5.82	123.31	112.77
1	B	206	ILE	N-CA-C	5.79	116.49	107.28
1	B	319	THR	CA-C-N	-5.78	114.94	120.83
1	B	319	THR	C-N-CA	-5.78	114.94	120.83
1	A	450	THR	CA-C-N	-5.77	114.81	120.52
1	A	450	THR	C-N-CA	-5.77	114.81	120.52
1	A	149	GLU	CG-CD-OE2	5.71	131.52	118.40
1	B	105	ALA	CA-C-N	-5.70	111.62	121.66
1	B	105	ALA	C-N-CA	-5.70	111.62	121.66
1	A	537	TYR	N-CA-CB	5.70	119.16	110.44
1	A	468	ARG	CA-C-N	-5.69	114.10	119.90
1	A	468	ARG	C-N-CA	-5.69	114.10	119.90
1	A	183	LEU	N-CA-C	-5.69	105.84	112.89
1	A	354	ASP	N-CA-C	5.67	119.46	112.54
1	B	461	PHE	N-CA-C	5.67	120.33	112.90
1	B	481	ASN	CA-C-N	5.67	130.62	122.40
1	B	481	ASN	C-N-CA	5.67	130.62	122.40
1	B	206	ILE	CB-CA-C	-5.66	103.63	110.99
1	A	196	MET	N-CA-C	-5.66	98.75	110.80
1	B	267	LYS	N-CA-C	5.64	122.81	110.80
1	B	528	GLY	CA-C-N	-5.63	114.13	119.76
1	B	528	GLY	C-N-CA	-5.63	114.13	119.76
1	A	47	SER	CA-C-O	5.58	128.01	121.87
1	B	81	VAL	O-C-N	-5.57	116.85	123.03
1	B	336	LEU	N-CA-C	5.54	120.04	113.28
1	A	388	PRO	CB-CA-C	-5.54	104.17	110.92
1	B	223	MET	N-CA-C	5.48	118.12	108.75
1	A	273	ILE	CB-CA-C	-5.45	104.90	112.04
1	B	82	TYR	CA-C-N	-5.44	112.74	122.32
1	B	82	TYR	C-N-CA	-5.44	112.74	122.32
1	B	446	PHE	CA-C-N	-5.43	114.10	119.92
1	B	446	PHE	C-N-CA	-5.43	114.10	119.92
1	A	250	TRP	N-CA-C	5.42	116.51	108.86
1	A	475	HIS	CA-C-N	5.42	128.18	122.11
1	A	475	HIS	C-N-CA	5.42	128.18	122.11
1	B	221	GLY	N-CA-C	5.37	120.14	111.38
1	A	270	ALA	N-CA-C	-5.36	105.43	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	576	ASN	CB-CG-OD1	5.35	131.51	120.80
1	A	249	LYS	CD-CE-NZ	-5.30	94.95	111.90
1	A	296	ASN	N-CA-C	-5.29	99.16	108.20
1	B	331	GLN	N-CA-CB	5.28	118.35	110.22
1	B	471	ALA	CA-C-N	-5.28	113.95	121.50
1	B	471	ALA	C-N-CA	-5.28	113.95	121.50
1	B	468	ARG	CA-C-N	-5.25	114.36	119.76
1	B	468	ARG	C-N-CA	-5.25	114.36	119.76
1	B	82	TYR	O-C-N	5.24	129.19	123.27
1	B	220	LYS	CA-C-N	-5.23	117.58	121.61
1	B	220	LYS	C-N-CA	-5.23	117.58	121.61
1	B	111	SER	N-CA-CB	-5.21	105.62	111.10
1	B	331	GLN	CB-CA-C	-5.18	101.04	110.63
1	B	576	ASN	N-CA-CB	-5.18	102.50	110.12
1	A	244	ILE	N-CA-C	-5.18	107.70	111.90
1	B	269	GLU	N-CA-C	-5.18	106.47	112.89
1	A	71	ALA	N-CA-C	5.17	117.75	110.14
1	A	356	TYR	N-CA-C	-5.17	105.54	111.07
1	B	183	LEU	N-CA-C	-5.17	105.82	111.82
1	B	389	PRO	N-CA-C	5.15	123.08	112.47
1	B	428	LEU	N-CA-C	5.12	117.44	110.88
1	B	502	LEU	CA-C-N	-5.10	111.09	121.18
1	B	502	LEU	C-N-CA	-5.10	111.09	121.18
1	A	287	VAL	N-CA-C	5.08	119.90	109.34
1	B	71	ALA	N-CA-C	5.07	118.38	110.32
1	B	576	ASN	CB-CA-C	-5.06	102.39	110.79
1	B	478	LEU	N-CA-C	-5.05	102.42	109.69
1	A	355	SER	CA-C-N	-5.04	113.89	120.44
1	A	355	SER	C-N-CA	-5.04	113.89	120.44
1	B	125	PRO	CA-N-CD	-5.03	104.95	112.00
1	B	179	GLY	CA-C-N	5.01	127.70	120.38
1	B	179	GLY	C-N-CA	5.01	127.70	120.38
1	B	452	ASP	O-C-N	5.01	125.38	121.47
1	B	440	TYR	N-CA-C	5.01	116.68	108.52
1	B	288	GLY	CA-C-N	-5.00	114.57	119.92
1	B	288	GLY	C-N-CA	-5.00	114.57	119.92

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	497	THR	CA

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	ASP	Mainchain
1	A	299	TYR	Mainchain
1	A	338	TRP	Mainchain
1	A	477	TRP	Mainchain
1	B	105	ALA	Mainchain
1	B	167	TYR	Sidechain
1	B	300	ALA	Mainchain
1	B	332	ASP	Sidechain
1	B	38	TRP	Mainchain
1	B	395	GLU	Mainchain
1	B	482	GLN	Mainchain
1	B	85	SER	Mainchain

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	4344	0	4293	215	0
1	B	4337	0	4282	217	0
2	A	53	0	31	11	0
2	B	53	0	31	11	0
3	A	102	0	0	4	1
3	B	74	0	0	2	1
All	All	8963	0	8637	436	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (436) 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:531:GLN:CB	1:A:531:GLN:CA	1.78	1.62
1:B:518:LEU:CB	1:B:518:LEU:CA	1.80	1.59
1:B:331:GLN:CB	1:B:331:GLN:CG	1.80	1.58
1:A:372:PHE:CZ	1:A:372:PHE:CE1	1.85	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:CB	1:A:50:ILE:CG1	1.85	1.55
1:A:47:SER:CA	1:A:47:SER:C	1.78	1.55
1:B:30:ILE:N	1:B:30:ILE:CA	1.67	1.55
1:A:268:GLU:CG	1:A:268:GLU:CB	1.82	1.53
1:A:50:ILE:CB	1:A:50:ILE:CA	1.84	1.53
1:B:128:VAL:CB	1:B:128:VAL:CA	1.88	1.52
1:B:105:ALA:C	1:B:105:ALA:CA	1.81	1.51
1:A:69:SER:C	1:A:70:LEU:N	1.67	1.50
1:B:179:GLY:C	1:B:180:ALA:N	1.70	1.50
1:A:531:GLN:CB	1:A:531:GLN:CG	1.88	1.49
1:B:300:ALA:CA	1:B:300:ALA:N	1.76	1.48
1:B:502:LEU:C	1:B:502:LEU:CA	1.85	1.48
1:B:296:ASN:C	1:B:296:ASN:CA	1.86	1.45
1:B:223:MET:HE3	1:B:225:TRP:CE2	1.50	1.45
1:B:331:GLN:CB	1:B:331:GLN:CA	1.92	1.44
1:B:223:MET:HE3	1:B:225:TRP:NE1	1.31	1.44
1:A:528:GLY:CA	1:A:528:GLY:C	1.92	1.43
1:B:355:SER:N	1:B:355:SER:CA	1.91	1.32
1:B:472:HIS:CA	1:B:472:HIS:N	1.91	1.32
1:B:446:PHE:O	1:B:446:PHE:CA	1.90	1.18
1:B:46:ARG:HD3	2:B:601:FAD:C7	1.74	1.17
1:B:223:MET:CE	1:B:225:TRP:CE2	2.30	1.14
1:B:392:THR:HG22	1:B:393:GLU:H	0.99	1.14
1:A:198:ILE:HG23	1:A:199:GLY:N	1.61	1.14
1:A:389:PRO:C	1:A:391:PRO:HD2	1.72	1.14
1:A:82:TYR:HE1	1:A:225:TRP:CE3	1.66	1.13
1:A:82:TYR:CE1	1:A:225:TRP:HE3	1.71	1.09
1:B:266:THR:HG21	1:B:270:ALA:HB2	1.33	1.09
1:B:398:GLU:O	1:B:402:ARG:NH1	1.86	1.09
1:A:212:LEU:HD11	1:A:283:ILE:HD13	1.34	1.07
1:B:446:PHE:O	1:B:446:PHE:C	0.81	1.06
1:B:36:ASN:OD1	2:B:601:FAD:O2B	1.74	1.06
1:B:223:MET:CE	1:B:225:TRP:NE1	2.19	1.06
1:B:223:MET:CE	1:B:225:TRP:CZ2	2.39	1.06
1:A:212:LEU:CD1	1:A:283:ILE:HD13	1.87	1.05
1:A:47:SER:C	1:A:47:SER:O	0.80	1.04
1:A:81:VAL:HG22	1:A:93:ARG:HD3	1.37	1.04
1:B:223:MET:HE1	1:B:225:TRP:CZ2	1.95	1.01
1:A:372:PHE:CZ	1:A:372:PHE:CD1	2.34	1.00
1:A:528:GLY:C	1:A:528:GLY:O	0.76	1.00
1:B:252:CYS:HB3	1:B:254:TRP:HZ3	1.22	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:HG22	1:A:290:ILE:HG12	1.45	0.98
1:A:387:LEU:HG	1:A:388:PRO:HD2	1.47	0.96
1:A:82:TYR:CE1	1:A:225:TRP:CE3	2.49	0.95
1:A:274:ILE:HA	1:A:277:ILE:HG22	1.48	0.95
1:B:354:ASP:C	1:B:355:SER:CA	2.39	0.95
1:A:198:ILE:HG23	1:A:199:GLY:H	1.18	0.94
1:B:392:THR:HG22	1:B:393:GLU:N	1.81	0.94
1:A:274:ILE:O	1:A:277:ILE:HG22	1.67	0.94
1:B:245:ARG:HG3	1:B:249:LYS:HD2	1.48	0.93
1:B:128:VAL:CA	1:B:128:VAL:CG2	2.46	0.92
1:B:128:VAL:CA	1:B:128:VAL:CG1	2.48	0.91
1:A:122:TYR:CE2	1:A:245:ARG:NH1	2.38	0.91
1:B:471:ALA:C	1:B:472:HIS:CA	2.44	0.90
1:B:266:THR:CG2	1:B:270:ALA:HB2	2.02	0.90
1:B:40:SER:HB2	3:B:741:HOH:O	1.72	0.89
1:A:295:ILE:HD13	1:A:318:HIS:O	1.71	0.88
1:A:198:ILE:CG2	1:A:199:GLY:N	2.36	0.88
1:A:531:GLN:CB	1:A:531:GLN:C	2.47	0.88
1:A:212:LEU:HD21	1:A:278:ILE:HD13	1.56	0.87
1:A:17:ALA:HB1	1:A:311:MET:HE3	1.55	0.87
1:A:77:MET:HB2	1:A:222:ASP:HB2	1.53	0.87
1:A:50:ILE:CG1	1:A:50:ILE:CA	2.52	0.87
1:A:50:ILE:CA	1:A:50:ILE:CG2	2.51	0.87
1:B:179:GLY:CA	1:B:180:ALA:N	2.38	0.86
1:A:212:LEU:HD12	1:A:283:ILE:HG21	1.58	0.86
1:A:47:SER:CA	1:A:48:HIS:N	2.38	0.86
1:B:206:ILE:HD12	1:B:254:TRP:HH2	1.39	0.85
1:A:50:ILE:CG1	1:A:50:ILE:CG2	2.51	0.85
1:A:212:LEU:CD1	1:A:283:ILE:HG21	2.07	0.85
1:B:105:ALA:C	1:B:105:ALA:CB	2.48	0.85
1:A:274:ILE:CA	1:A:277:ILE:HG22	2.06	0.84
1:B:105:ALA:CA	1:B:106:GLU:N	2.38	0.84
1:A:268:GLU:CG	1:A:268:GLU:CA	2.56	0.83
1:A:69:SER:CA	1:A:70:LEU:N	2.42	0.83
1:A:197:GLY:O	1:A:198:ILE:HG22	1.78	0.83
1:A:531:GLN:CA	1:A:531:GLN:CG	2.56	0.83
1:B:446:PHE:O	1:B:447:PRO:N	2.08	0.83
1:A:528:GLY:CA	1:A:529:PRO:N	2.42	0.82
1:B:296:ASN:CA	1:B:297:GLN:N	2.42	0.82
1:B:355:SER:O	1:B:359:GLU:HB2	1.79	0.82
1:A:113:SER:C	1:A:114:ARG:HG2	2.05	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:VAL:HB	1:A:117:ASP:HB3	1.62	0.81
1:A:274:ILE:HA	1:A:277:ILE:CG2	2.11	0.81
1:A:496:PHE:HB3	1:A:522:LEU:CD1	2.11	0.81
1:B:557:ASP:O	1:B:558:MET:HB2	1.79	0.81
1:B:382:PHE:O	1:B:383:GLU:C	2.20	0.81
1:B:511:ALA:HB1	1:B:522:LEU:HD22	1.63	0.81
1:A:36:ASN:OD1	2:A:601:FAD:O2B	1.99	0.80
1:B:115:TYR:OH	1:B:435:GLU:OE2	1.98	0.80
1:B:39:ARG:HG2	1:B:39:ARG:HH11	1.46	0.80
1:B:518:LEU:CA	1:B:518:LEU:CG	2.60	0.80
1:B:300:ALA:N	1:B:300:ALA:CB	2.45	0.80
1:A:220:LYS:HG2	1:A:247:TRP:HZ2	1.47	0.79
1:B:491:CYS:HB2	1:B:558:MET:HE1	1.64	0.79
1:B:86:LEU:CD2	1:B:212:LEU:HD13	2.13	0.79
1:B:204:ILE:HD11	1:B:264:GLU:CB	2.13	0.79
1:B:117:ASP:OD2	1:B:222:ASP:OD2	2.01	0.79
1:B:331:GLN:CG	1:B:331:GLN:CA	2.61	0.79
1:B:252:CYS:HB3	1:B:254:TRP:CZ3	2.15	0.79
1:A:387:LEU:CG	1:A:388:PRO:HD2	2.14	0.78
1:A:113:SER:O	1:A:114:ARG:HG2	1.83	0.78
1:B:227:PHE:CZ	1:B:381:VAL:HG11	2.18	0.78
1:B:105:ALA:CA	1:B:105:ALA:O	2.32	0.78
1:B:299:TYR:CZ	1:B:365:LYS:HG3	2.19	0.77
1:B:331:GLN:CB	1:B:331:GLN:CD	2.57	0.77
1:A:274:ILE:C	1:A:277:ILE:HG22	2.09	0.77
1:A:388:PRO:HG2	1:A:391:PRO:HD3	1.65	0.77
1:B:197:GLY:O	1:B:198:ILE:O	2.01	0.77
1:A:50:ILE:CB	1:A:50:ILE:C	2.58	0.77
1:B:223:MET:HE1	1:B:225:TRP:HZ2	1.47	0.77
1:B:378:PHE:H	1:B:379:PRO:HD2	1.49	0.77
1:B:264:GLU:O	1:B:265:ILE:HG12	1.85	0.76
1:B:392:THR:CG2	1:B:393:GLU:H	1.85	0.76
1:B:492:GLY:O	3:B:701:HOH:O	2.02	0.76
1:A:47:SER:C	1:A:47:SER:N	2.43	0.76
1:B:418:ARG:O	1:B:418:ARG:HD3	1.86	0.75
1:B:557:ASP:O	1:B:558:MET:CB	2.33	0.75
1:A:223:MET:HE3	1:A:225:TRP:NE1	2.02	0.75
1:A:389:PRO:C	1:A:391:PRO:CD	2.56	0.74
1:B:381:VAL:O	1:B:384:ALA:HB3	1.87	0.74
1:B:377:THR:O	1:B:424:THR:HG22	1.86	0.74
1:B:502:LEU:CA	1:B:502:LEU:O	2.34	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:LEU:CB	1:B:518:LEU:C	2.59	0.74
1:B:46:ARG:CD	2:B:601:FAD:C7	2.62	0.74
1:B:378:PHE:H	1:B:379:PRO:CD	2.00	0.74
1:B:154:VAL:HG21	1:B:174:ILE:HG13	1.69	0.73
1:A:417:LEU:HG	1:A:421:MET:HE2	1.68	0.73
1:B:30:ILE:N	1:B:30:ILE:CB	2.48	0.73
1:B:502:LEU:CA	1:B:503:SER:N	2.42	0.73
1:A:357:ASP:O	1:A:361:SER:HB2	1.89	0.73
1:B:204:ILE:HD11	1:B:264:GLU:HB2	1.70	0.72
1:A:496:PHE:CB	1:A:522:LEU:CD1	2.68	0.72
1:A:69:SER:C	1:A:70:LEU:CA	2.61	0.71
1:B:514:VAL:HG12	1:B:518:LEU:HD12	1.72	0.71
1:A:390:ALA:N	1:A:391:PRO:CD	2.54	0.71
1:A:254:TRP:HD1	1:A:255:GLY:O	1.74	0.70
1:B:378:PHE:HB2	1:B:379:PRO:HD3	1.73	0.70
1:B:30:ILE:N	1:B:30:ILE:C	2.46	0.70
1:B:82:TYR:CD1	1:B:227:PHE:CZ	2.79	0.70
1:A:389:PRO:O	1:A:391:PRO:HD2	1.91	0.70
1:B:300:ALA:N	1:B:300:ALA:C	2.45	0.70
1:B:575:LEU:O	1:B:579:VAL:HG23	1.92	0.70
1:A:481:ASN:O	1:A:482:GLN:HB2	1.91	0.69
1:A:295:ILE:HD11	1:A:318:HIS:N	2.08	0.69
1:A:220:LYS:CG	1:A:247:TRP:HZ2	2.06	0.69
1:A:528:GLY:CA	1:A:528:GLY:O	2.40	0.69
2:A:601:FAD:H1'1	3:A:726:HOH:O	1.92	0.69
1:B:60:ASP:OD2	1:B:334:TYR:OH	2.09	0.68
1:B:378:PHE:N	1:B:379:PRO:CD	2.56	0.68
1:A:47:SER:CA	1:A:47:SER:O	2.36	0.68
1:A:45:PRO:HB2	1:A:242:ARG:HH22	1.58	0.68
1:B:452:ASP:OD1	1:B:453:PRO:HD2	1.95	0.67
1:A:212:LEU:HD11	1:A:283:ILE:CD1	2.18	0.67
1:B:278:ILE:HG22	1:B:280:THR:HG22	1.75	0.67
1:B:269:GLU:O	1:B:272:LYS:HB3	1.95	0.67
1:B:204:ILE:HD11	1:B:264:GLU:HB3	1.77	0.67
1:B:266:THR:HG21	1:B:270:ALA:CB	2.19	0.67
2:A:601:FAD:O2	3:A:702:HOH:O	2.13	0.66
1:B:20:MET:HG2	1:B:330:VAL:HG13	1.77	0.66
1:B:382:PHE:C	1:B:384:ALA:N	2.50	0.66
1:B:46:ARG:HD3	2:B:601:FAD:C6	2.24	0.66
1:B:331:GLN:CB	1:B:331:GLN:C	2.68	0.66
1:A:515:SER:HB2	1:A:520:ILE:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:VAL:HG21	1:A:174:ILE:HG13	1.76	0.66
1:B:479:THR:OG1	1:B:536:THR:OG1	2.08	0.66
1:B:206:ILE:CD1	1:B:254:TRP:HH2	2.08	0.65
1:B:13:GLY:HA2	2:B:601:FAD:O4B	1.96	0.65
1:B:223:MET:CE	1:B:225:TRP:HE1	2.01	0.65
1:B:206:ILE:HD12	1:B:254:TRP:CH2	2.28	0.65
1:A:212:LEU:HD21	1:A:278:ILE:CD1	2.26	0.65
1:B:46:ARG:HD3	2:B:601:FAD:C7M	2.26	0.64
1:B:179:GLY:O	1:B:180:ALA:N	2.26	0.64
1:A:210:ALA:O	1:A:248:ASN:HA	1.98	0.63
1:B:58:LEU:HD13	1:B:67:ALA:HB2	1.80	0.63
1:B:355:SER:O	1:B:359:GLU:CB	2.46	0.63
1:A:89:GLU:OE1	1:A:400:LEU:CD2	2.47	0.63
1:A:223:MET:HE3	1:A:225:TRP:HE1	1.63	0.63
1:A:278:ILE:HG21	1:A:283:ILE:HD12	1.80	0.63
1:B:296:ASN:C	1:B:296:ASN:N	2.57	0.63
1:B:296:ASN:C	1:B:296:ASN:CB	2.71	0.63
1:B:510:GLU:O	1:B:514:VAL:HG23	1.99	0.62
1:A:198:ILE:CG2	1:A:199:GLY:H	1.96	0.62
1:A:89:GLU:OE1	1:A:400:LEU:HD22	1.99	0.62
1:B:386:SER:HB3	1:B:402:ARG:HH21	1.64	0.62
1:B:417:LEU:HG	1:B:421:MET:HE2	1.81	0.62
1:A:50:ILE:HG23	1:A:50:ILE:CD1	2.30	0.62
1:A:121:LEU:HD23	1:A:122:TYR:CE1	2.35	0.62
1:A:157:ARG:HG3	1:A:157:ARG:HH11	1.65	0.61
1:B:206:ILE:CD1	1:B:254:TRP:CH2	2.83	0.61
1:A:295:ILE:HD11	1:A:318:HIS:H	1.65	0.61
1:B:397:ALA:O	1:B:401:VAL:HG23	2.00	0.61
1:A:42:SER:HB2	1:A:124:GLU:OE1	1.99	0.61
1:A:212:LEU:CG	1:A:283:ILE:HD13	2.29	0.61
1:A:243:MET:HE2	1:A:246:PRO:HB3	1.81	0.61
1:A:178:ASP:OD1	1:A:182:SER:OG	2.16	0.61
1:B:207:GLU:HG2	1:B:251:ILE:HD12	1.82	0.61
1:A:82:TYR:HE1	1:A:225:TRP:HE3	0.83	0.61
1:B:336:LEU:O	1:B:336:LEU:HG	2.01	0.61
1:B:382:PHE:O	1:B:384:ALA:N	2.34	0.60
1:A:20:MET:HG2	1:A:330:VAL:HG13	1.82	0.60
1:A:496:PHE:CB	1:A:522:LEU:HD12	2.31	0.60
1:A:50:ILE:N	1:A:50:ILE:HG12	2.15	0.60
1:A:50:ILE:CB	1:A:50:ILE:CD1	2.76	0.60
1:A:208:PHE:HD1	1:A:285:VAL:HG13	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:PHE:CD1	1:A:285:VAL:HG13	2.37	0.60
1:A:392:THR:OG1	1:A:393:GLU:N	2.33	0.60
1:B:237:GLY:HA2	1:B:391:PRO:HG3	1.84	0.60
1:B:48:HIS:NE2	1:B:242:ARG:HD2	2.16	0.60
1:A:196:MET:HG3	1:A:196:MET:O	2.02	0.59
1:A:274:ILE:O	1:A:277:ILE:CG2	2.49	0.59
1:B:355:SER:O	1:B:359:GLU:HG3	2.02	0.59
1:B:61:ILE:O	1:B:134:ARG:NH2	2.33	0.59
1:A:227:PHE:CD2	1:A:382:PHE:HE1	2.21	0.59
1:A:254:TRP:CH2	1:A:273:ILE:HG21	2.38	0.59
1:A:77:MET:CB	1:A:222:ASP:HB2	2.30	0.59
1:B:341:ALA:O	1:B:345:LYS:HG3	2.03	0.58
1:B:363:VAL:O	1:B:367:ILE:HG23	2.03	0.58
1:A:238:VAL:HB	1:A:378:PHE:CZ	2.38	0.58
1:A:472:HIS:CD2	1:A:558:MET:HB3	2.38	0.58
1:A:37:ARG:HD3	1:A:143:GLU:HB3	1.84	0.58
2:A:601:FAD:H1'2	3:A:747:HOH:O	2.03	0.58
1:A:111:SER:OG	1:A:112:PRO:HD2	2.03	0.57
1:B:225:TRP:CH2	1:B:378:PHE:CE1	2.92	0.57
1:A:227:PHE:CD2	1:A:382:PHE:CE1	2.92	0.57
1:A:206:ILE:O	1:A:251:ILE:HA	2.04	0.57
1:B:555:ARG:NH2	1:B:557:ASP:OD2	2.36	0.57
1:A:557:ASP:O	1:A:558:MET:HB2	2.02	0.57
1:B:473:LEU:HD23	1:B:558:MET:CE	2.35	0.57
1:B:473:LEU:HD23	1:B:558:MET:HE2	1.85	0.57
1:A:409:GLU:O	1:A:413:ARG:HG3	2.03	0.57
1:B:225:TRP:CZ3	1:B:378:PHE:CE1	2.93	0.57
1:A:514:VAL:HG12	1:A:514:VAL:O	2.05	0.57
1:B:46:ARG:HD3	2:B:601:FAD:C8	2.31	0.57
1:B:224:TYR:O	1:B:226:MET:HE2	2.05	0.57
1:A:59:ARG:HG3	1:A:64:GLU:OE1	2.05	0.56
1:A:388:PRO:HG2	1:A:391:PRO:CD	2.34	0.56
1:A:486:SER:O	1:A:487:THR:C	2.48	0.56
1:B:178:ASP:OD2	1:B:184:VAL:HG23	2.05	0.56
1:B:386:SER:CB	1:B:402:ARG:HH21	2.18	0.56
1:A:528:GLY:C	1:A:534:VAL:HG13	2.31	0.56
1:A:121:LEU:CD2	1:A:122:TYR:CE1	2.89	0.56
1:A:441:VAL:O	1:A:442:SER:HB3	2.05	0.56
1:B:382:PHE:O	1:B:385:LEU:N	2.39	0.56
1:A:177:ALA:HB2	1:A:311:MET:HE2	1.87	0.56
1:B:266:THR:HG23	1:B:269:GLU:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:PHE:HB3	1:A:522:LEU:HD11	1.86	0.56
1:B:58:LEU:HA	1:B:61:ILE:HD11	1.87	0.56
1:B:294:THR:C	1:B:295:ILE:HG13	2.31	0.56
1:B:150:ASP:OD2	1:B:170:ARG:NH1	2.39	0.55
1:B:514:VAL:CG1	1:B:518:LEU:HD12	2.34	0.55
1:A:496:PHE:HB3	1:A:522:LEU:HD12	1.87	0.55
1:B:199:GLY:O	1:B:200:ASP:C	2.48	0.55
1:B:553:LEU:HB3	1:B:562:PHE:HB3	1.89	0.55
1:A:402:ARG:HE	1:A:413:ARG:NH2	2.05	0.55
1:B:441:VAL:O	1:B:442:SER:HB3	2.06	0.55
1:B:555:ARG:HB2	1:B:557:ASP:OD1	2.07	0.55
1:B:212:LEU:HD23	1:B:283:ILE:HD13	1.89	0.55
1:B:58:LEU:HD13	1:B:67:ALA:CB	2.36	0.55
1:B:245:ARG:CG	1:B:249:LYS:HD2	2.29	0.54
1:A:220:LYS:HG2	1:A:247:TRP:CZ2	2.36	0.54
1:B:238:VAL:HG12	1:B:238:VAL:O	2.07	0.54
1:A:531:GLN:CB	1:A:531:GLN:N	2.64	0.54
1:B:150:ASP:OD1	1:B:152:ASP:N	2.19	0.54
1:B:446:PHE:O	1:B:446:PHE:CB	2.52	0.54
1:A:227:PHE:CE2	1:A:382:PHE:HE1	2.26	0.54
1:A:528:GLY:CA	1:A:529:PRO:CD	2.85	0.54
1:B:169:VAL:HG13	1:B:169:VAL:O	2.08	0.54
1:B:359:GLU:O	1:B:360:ARG:HD2	2.08	0.54
1:B:398:GLU:O	1:B:398:GLU:HG3	2.08	0.54
1:B:357:ASP:O	1:B:361:SER:HB2	2.08	0.53
1:B:209:SER:HB2	1:B:286:GLU:HB2	1.90	0.53
1:B:150:ASP:OD1	1:B:151:GLN:N	2.41	0.53
1:A:278:ILE:HG21	1:A:283:ILE:CD1	2.38	0.53
1:A:108:GLU:HG3	1:A:114:ARG:CZ	2.39	0.53
1:A:271:LYS:HA	1:A:274:ILE:HD12	1.90	0.53
1:B:46:ARG:CD	2:B:601:FAD:C8	2.87	0.53
1:B:266:THR:HG22	1:B:267:LYS:N	2.22	0.53
1:B:402:ARG:HG3	1:B:402:ARG:HH11	1.74	0.53
1:A:7:THR:O	1:A:171:ALA:HA	2.09	0.53
1:A:239:ALA:O	1:A:240:ALA:HB2	2.09	0.53
1:B:282:GLU:HA	1:B:282:GLU:OE1	2.09	0.53
1:A:145:LEU:HD11	1:A:159:LEU:HB2	1.91	0.52
1:B:16:PRO:HG2	1:B:120:GLN:HE21	1.74	0.52
1:B:544:SER:O	1:B:545:GLU:HB2	2.08	0.52
1:A:475:HIS:CE1	1:A:486:SER:HG	2.22	0.52
1:A:299:TYR:CZ	1:A:365:LYS:HG3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:PHE:HB2	1:A:522:LEU:CD1	2.38	0.52
1:B:202:GLY:HA3	1:B:294:THR:HG22	1.91	0.52
1:A:28:LEU:O	1:A:345:LYS:NZ	2.34	0.52
1:B:355:SER:O	1:B:359:GLU:CG	2.57	0.52
1:A:338:TRP:CE2	1:A:339:LYS:HG3	2.45	0.52
1:A:486:SER:O	1:A:488:LEU:N	2.43	0.52
1:B:28:LEU:HD21	1:B:494:GLY:HA3	1.92	0.52
1:B:75:GLU:OE1	1:B:75:GLU:N	2.43	0.52
1:B:225:TRP:HH2	1:B:378:PHE:CZ	2.27	0.52
1:A:47:SER:C	1:A:47:SER:CB	2.74	0.52
1:B:39:ARG:HG2	1:B:39:ARG:NH1	2.19	0.52
1:B:46:ARG:HB2	1:B:120:GLN:OE1	2.10	0.52
1:B:76:TYR:N	1:B:76:TYR:CD1	2.78	0.52
1:A:53:ARG:NH1	1:A:438:GLN:OE1	2.43	0.51
1:A:326:LEU:C	1:A:326:LEU:HD23	2.36	0.51
1:A:445:VAL:O	1:A:447:PRO:HD3	2.11	0.51
1:B:43:PRO:O	1:B:121:LEU:HD13	2.11	0.51
1:B:128:VAL:CB	1:B:128:VAL:N	2.64	0.51
1:B:80:HIS:NE2	1:B:223:MET:HE2	2.26	0.51
1:B:334:TYR:CE2	1:B:557:ASP:HA	2.46	0.51
1:A:50:ILE:CA	1:A:50:ILE:HG12	2.37	0.51
1:A:378:PHE:CD1	1:A:378:PHE:C	2.89	0.51
1:A:13:GLY:HA2	2:A:601:FAD:O4B	2.11	0.51
1:A:227:PHE:CE2	1:A:382:PHE:CE1	2.99	0.50
1:B:39:ARG:HH11	1:B:39:ARG:CG	2.16	0.50
1:A:122:TYR:HE2	1:A:245:ARG:NH1	1.99	0.50
1:A:178:ASP:OD2	1:A:184:VAL:HG23	2.11	0.50
1:B:76:TYR:N	1:B:76:TYR:HD1	2.10	0.50
1:B:384:ALA:C	1:B:386:SER:H	2.18	0.50
1:A:336:LEU:HG	1:A:336:LEU:O	2.10	0.50
1:B:325:GLY:O	1:B:329:SER:OG	2.24	0.50
1:A:178:ASP:C	2:A:601:FAD:H52A	2.36	0.50
1:A:418:ARG:O	1:A:418:ARG:HD3	2.12	0.50
1:A:270:ALA:HA	1:A:273:ILE:HG13	1.94	0.50
1:B:502:LEU:C	1:B:502:LEU:CB	2.76	0.50
1:B:518:LEU:HB2	1:B:520:ILE:HG22	1.93	0.49
1:A:157:ARG:HG3	1:A:157:ARG:NH1	2.28	0.49
1:A:531:GLN:HB3	3:A:732:HOH:O	2.12	0.49
1:B:278:ILE:HG22	1:B:278:ILE:O	2.11	0.49
1:B:402:ARG:NH1	1:B:402:ARG:HG3	2.28	0.49
1:A:295:ILE:HG23	1:A:295:ILE:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ARG:NH1	1:B:39:ARG:CG	2.72	0.49
1:B:113:SER:O	1:B:114:ARG:NH1	2.46	0.49
1:A:107:HIS:CE1	1:A:115:TYR:CD2	3.00	0.49
1:A:15:GLY:HA3	2:A:601:FAD:O1A	2.12	0.49
1:B:82:TYR:HD1	1:B:227:PHE:CZ	2.27	0.49
1:A:388:PRO:HG2	1:A:388:PRO:O	2.07	0.49
1:B:299:TYR:CE1	1:B:365:LYS:HG3	2.47	0.49
1:B:338:TRP:CZ2	1:B:339:LYS:HE3	2.48	0.49
1:A:50:ILE:CG2	1:A:50:ILE:CD1	2.89	0.49
1:A:178:ASP:OD1	1:A:178:ASP:N	2.39	0.49
1:A:397:ALA:O	1:A:401:VAL:HG23	2.13	0.49
1:A:45:PRO:HB2	1:A:242:ARG:NH2	2.27	0.48
1:A:274:ILE:O	1:A:277:ILE:N	2.46	0.48
1:A:220:LYS:CG	1:A:247:TRP:CZ2	2.93	0.48
1:A:472:HIS:ND1	1:A:473:LEU:O	2.45	0.48
1:A:472:HIS:NE2	1:A:558:MET:HB3	2.28	0.48
1:A:238:VAL:O	1:A:238:VAL:HG13	2.14	0.48
1:B:86:LEU:HD21	1:B:212:LEU:HD13	1.92	0.48
1:A:47:SER:HB3	1:A:120:GLN:HG3	1.96	0.48
1:B:197:GLY:C	1:B:198:ILE:O	2.57	0.48
1:A:238:VAL:HB	1:A:378:PHE:CE2	2.49	0.48
1:B:386:SER:HB3	1:B:402:ARG:NH2	2.28	0.48
1:A:378:PHE:HB3	1:A:379:PRO:CD	2.44	0.47
1:A:16:PRO:HD2	2:A:601:FAD:O2P	2.14	0.47
1:A:46:ARG:C	1:A:47:SER:C	2.83	0.47
1:A:528:GLY:C	1:A:528:GLY:N	2.69	0.47
1:B:378:PHE:N	1:B:379:PRO:HD2	2.19	0.47
1:A:246:PRO:HA	1:A:247:TRP:HA	1.58	0.47
1:B:159:LEU:HD12	1:B:160:ASP:N	2.29	0.47
1:A:89:GLU:OE1	1:A:400:LEU:HD21	2.14	0.46
1:A:242:ARG:HB3	1:A:251:ILE:HG22	1.97	0.46
1:B:128:VAL:HG12	1:B:128:VAL:C	2.40	0.46
1:A:55:MET:HE3	1:A:64:GLU:HG3	1.96	0.46
1:B:266:THR:CG2	1:B:267:LYS:N	2.78	0.46
1:A:553:LEU:HB3	1:A:562:PHE:HB3	1.98	0.46
1:B:46:ARG:CD	2:B:601:FAD:C6	2.90	0.46
1:A:42:SER:CB	1:A:124:GLU:OE1	2.62	0.46
1:A:46:ARG:O	1:A:242:ARG:NH1	2.43	0.45
1:B:13:GLY:HA3	1:B:177:ALA:O	2.16	0.45
1:A:269:GLU:O	1:A:272:LYS:HB2	2.16	0.45
1:A:378:PHE:HB3	1:A:379:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ILE:CD1	1:B:264:GLU:HB3	2.44	0.45
1:A:121:LEU:HG	1:A:122:TYR:CD1	2.52	0.45
1:A:212:LEU:HG	1:A:283:ILE:HD13	1.98	0.45
1:B:225:TRP:CH2	1:B:378:PHE:CZ	3.04	0.45
1:A:324:LEU:O	1:A:328:THR:OG1	2.33	0.45
1:B:485:ILE:HD13	1:B:490:LEU:CD1	2.46	0.45
1:A:509:HIS:O	1:A:510:GLU:C	2.58	0.45
1:B:16:PRO:HD2	2:B:601:FAD:O2P	2.16	0.45
1:B:418:ARG:HD3	1:B:418:ARG:C	2.38	0.45
1:A:242:ARG:HB3	1:A:251:ILE:CG2	2.47	0.44
1:B:128:VAL:CG1	1:B:128:VAL:C	2.89	0.44
1:A:107:HIS:HE1	1:A:115:TYR:CD2	2.36	0.44
1:B:518:LEU:HD21	1:B:580:LYS:HG2	1.98	0.44
1:A:322:GLY:O	1:A:323:GLY:C	2.61	0.44
1:A:351:THR:O	1:A:352:LEU:C	2.58	0.44
1:B:55:MET:HE3	1:B:64:GLU:HG3	1.98	0.44
1:A:123:PHE:CD1	1:A:123:PHE:C	2.96	0.44
1:A:295:ILE:HD13	1:A:318:HIS:C	2.38	0.44
1:A:553:LEU:HD23	1:A:562:PHE:HB3	2.00	0.44
1:B:300:ALA:HB1	1:B:302:ARG:O	2.17	0.44
1:A:486:SER:C	1:A:488:LEU:N	2.76	0.43
1:A:46:ARG:HG2	2:A:601:FAD:C5X	2.48	0.43
1:B:267:LYS:HB3	1:B:268:GLU:H	1.60	0.43
1:A:245:ARG:HB2	1:A:249:LYS:HB2	2.00	0.43
1:B:311:MET:HE1	1:B:333:ALA:HA	2.00	0.43
1:A:373:LYS:O	1:A:376:SER:OG	2.36	0.43
1:B:220:LYS:HG2	1:B:247:TRP:CZ2	2.54	0.43
1:B:486:SER:O	1:B:487:THR:C	2.61	0.43
1:B:297:GLN:HG2	1:B:318:HIS:HA	2.01	0.43
1:A:150:ASP:CG	1:A:170:ARG:HH22	2.27	0.43
1:A:267:LYS:C	1:A:269:GLU:N	2.74	0.43
1:A:378:PHE:H	1:A:379:PRO:HD2	1.84	0.43
1:A:55:MET:HB3	1:A:113:SER:HB3	2.01	0.43
1:A:311:MET:HA	1:A:315:VAL:HG21	2.01	0.43
1:B:220:LYS:HG2	1:B:247:TRP:HZ2	1.83	0.43
1:A:178:ASP:CG	1:A:182:SER:OG	2.61	0.43
1:B:379:PRO:C	1:B:381:VAL:N	2.76	0.43
1:B:324:LEU:O	1:B:328:THR:OG1	2.34	0.42
1:A:17:ALA:CB	1:A:311:MET:HE3	2.39	0.42
1:A:69:SER:N	1:A:70:LEU:N	2.67	0.42
1:A:315:VAL:HG23	1:A:316:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:MET:SD	1:B:245:ARG:C	3.03	0.42
1:A:295:ILE:CD1	1:A:318:HIS:O	2.56	0.42
1:A:178:ASP:HA	2:A:601:FAD:H52A	2.02	0.41
1:B:13:GLY:HA2	2:B:601:FAD:C1B	2.49	0.41
1:B:225:TRP:HH2	1:B:378:PHE:CE1	2.38	0.41
1:A:295:ILE:CD1	1:A:318:HIS:N	2.79	0.41
1:B:243:MET:HB3	1:B:243:MET:HE3	1.78	0.41
1:A:378:PHE:N	1:A:379:PRO:HD2	2.35	0.41
1:A:312:GLY:C	1:A:314:ALA:N	2.77	0.41
2:A:601:FAD:O4'	2:A:601:FAD:O2'	2.28	0.41
1:B:491:CYS:CB	1:B:558:MET:HE1	2.44	0.41
1:A:311:MET:HB3	1:A:356:TYR:OH	2.20	0.41
1:A:378:PHE:O	1:A:379:PRO:C	2.62	0.41
1:B:60:ASP:OD1	1:B:492:GLY:O	2.38	0.41
1:B:223:MET:HE3	1:B:225:TRP:CD1	2.34	0.41
1:B:216:CYS:O	1:B:217:GLU:C	2.63	0.41
1:B:223:MET:SD	1:B:225:TRP:NE1	2.93	0.40
1:A:574:GLN:O	1:A:575:LEU:C	2.62	0.40
1:A:385:LEU:O	1:A:386:SER:C	2.64	0.40
1:B:202:GLY:HA2	1:B:294:THR:HA	2.01	0.40
1:B:275:HIS:ND1	1:B:281:ASP:HB2	2.36	0.40
1:A:55:MET:O	1:A:56:GLU:C	2.65	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:772:HOH:O	3:B:755:HOH:O[4_555]	2.13	0.07

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	560/581 (96%)	503 (90%)	52 (9%)	5 (1%)	14	37
1	B	559/581 (96%)	507 (91%)	49 (9%)	3 (0%)	24	52
All	All	1119/1162 (96%)	1010 (90%)	101 (9%)	8 (1%)	18	44

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	198	ILE
1	A	198	ILE
1	A	487	THR
1	A	43	PRO
1	A	390	ALA
1	A	217	GLU
1	B	391	PRO
1	B	238	VAL

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	452/462 (98%)	429 (95%)	23 (5%)	21	50
1	B	451/462 (98%)	424 (94%)	27 (6%)	17	43
All	All	903/924 (98%)	853 (94%)	50 (6%)	19	47

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	70	LEU
1	A	124	GLU
1	A	198	ILE
1	A	207	GLU
1	A	212	LEU
1	A	220	LYS
1	A	252	CYS

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Mol	Chain	Res	Type
1	A	273	ILE
1	A	275	HIS
1	A	283	ILE
1	A	311	MET
1	A	317	ARG
1	A	319	THR
1	A	380	PRO
1	A	387	LEU
1	A	392	THR
1	A	396	MET
1	A	398	GLU
1	A	484	ARG
1	A	497	THR
1	A	537	TYR
1	A	565	LYS
1	B	6	GLU
1	B	46	ARG
1	B	53	ARG
1	B	90	GLU
1	B	166	GLU
1	B	195	GLN
1	B	204	ILE
1	B	248	ASN
1	B	251	ILE
1	B	252	CYS
1	B	267	LYS
1	B	295	ILE
1	B	317	ARG
1	B	361	SER
1	B	367	ILE
1	B	369	GLU
1	B	386	SER
1	B	414	ARG
1	B	419	LYS
1	B	436	LEU
1	B	482	GLN
1	B	484	ARG
1	B	485	ILE
1	B	493	LYS
1	B	495	ARG
1	B	503	SER
1	B	558	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	HIS
1	A	316	HIS
1	A	509	HIS
1	A	513	GLN
1	B	52	GLN

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	A	601	-	58,58,58	1.48	8 (13%)	85,89,89	1.56	15 (17%)
2	FAD	B	601	-	58,58,58	1.48	9 (15%)	85,89,89	1.56	15 (17%)

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	601	-	-	7/34/50/50	0/6/6/6
2	FAD	B	601	-	-	8/34/50/50	0/6/6/6

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C9A-C5X	5.29	1.49	1.41
2	B	601	FAD	C9A-C5X	5.24	1.49	1.41
2	B	601	FAD	C5A-C4A	4.75	1.47	1.39
2	A	601	FAD	C5A-C4A	4.75	1.47	1.39
2	B	601	FAD	C8-C7	3.40	1.49	1.40
2	A	601	FAD	C8-C7	3.39	1.49	1.40
2	B	601	FAD	C5A-C6A	2.77	1.48	1.41
2	A	601	FAD	C5A-C6A	2.74	1.48	1.41
2	B	601	FAD	C4-N3	-2.43	1.34	1.38
2	A	601	FAD	C8A-N7A	2.41	1.36	1.31
2	A	601	FAD	C4-N3	-2.41	1.34	1.38
2	B	601	FAD	C8A-N7A	2.38	1.36	1.31
2	A	601	FAD	C5A-N7A	-2.25	1.35	1.39
2	B	601	FAD	C4X-N5	2.24	1.35	1.30
2	A	601	FAD	C4X-N5	2.24	1.35	1.30
2	B	601	FAD	C5A-N7A	-2.24	1.35	1.39
2	B	601	FAD	C5X-N5	-2.01	1.35	1.39

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C5A-C4A-N3A	-5.86	118.65	126.72
2	A	601	FAD	C5A-C4A-N3A	-5.83	118.69	126.72
2	B	601	FAD	N3A-C4A-N9A	4.64	135.06	127.17
2	A	601	FAD	N3A-C4A-N9A	4.60	134.99	127.17
2	B	601	FAD	C2A-N3A-C4A	3.70	120.88	111.83
2	A	601	FAD	C2A-N3A-C4A	3.69	120.84	111.83
2	A	601	FAD	C4A-C5A-N7A	-3.48	106.60	110.58
2	B	601	FAD	C4A-C5A-N7A	-3.47	106.62	110.58
2	B	601	FAD	N3A-C2A-N1A	-3.21	123.72	128.58
2	A	601	FAD	N3A-C2A-N1A	-3.21	123.73	128.58
2	B	601	FAD	C4-C4X-N5	2.84	122.14	118.21
2	A	601	FAD	C4-C4X-N5	2.83	122.12	118.21
2	B	601	FAD	C4A-N9A-C8A	2.64	108.51	105.74
2	A	601	FAD	C4A-N9A-C8A	2.62	108.49	105.74
2	A	601	FAD	C3B-C2B-C1B	2.57	106.32	101.46
2	A	601	FAD	C5A-N7A-C8A	2.55	107.45	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C5A-N7A-C8A	2.54	107.44	103.45
2	B	601	FAD	C3B-C2B-C1B	2.54	106.27	101.46
2	B	601	FAD	C4X-C10-N1	-2.46	118.55	124.59
2	A	601	FAD	C4X-C10-N1	-2.46	118.56	124.59
2	B	601	FAD	O4-C4-C4X	-2.18	120.79	126.53
2	A	601	FAD	O4-C4-C4X	-2.17	120.80	126.53
2	B	601	FAD	C4X-C10-N10	2.12	119.51	116.48
2	B	601	FAD	C10-N1-C2	2.11	121.41	116.85
2	A	601	FAD	C10-N1-C2	2.10	121.40	116.85
2	A	601	FAD	C4X-C10-N10	2.09	119.47	116.48
2	A	601	FAD	C6A-C5A-N7A	2.08	136.10	132.09
2	B	601	FAD	C6A-C5A-N7A	2.07	136.09	132.09
2	A	601	FAD	C4X-C4-N3	2.05	118.47	113.25
2	B	601	FAD	C4X-C4-N3	2.03	118.43	113.25

There are no chirality outliers.

All (15) torsion outliers are listed below:

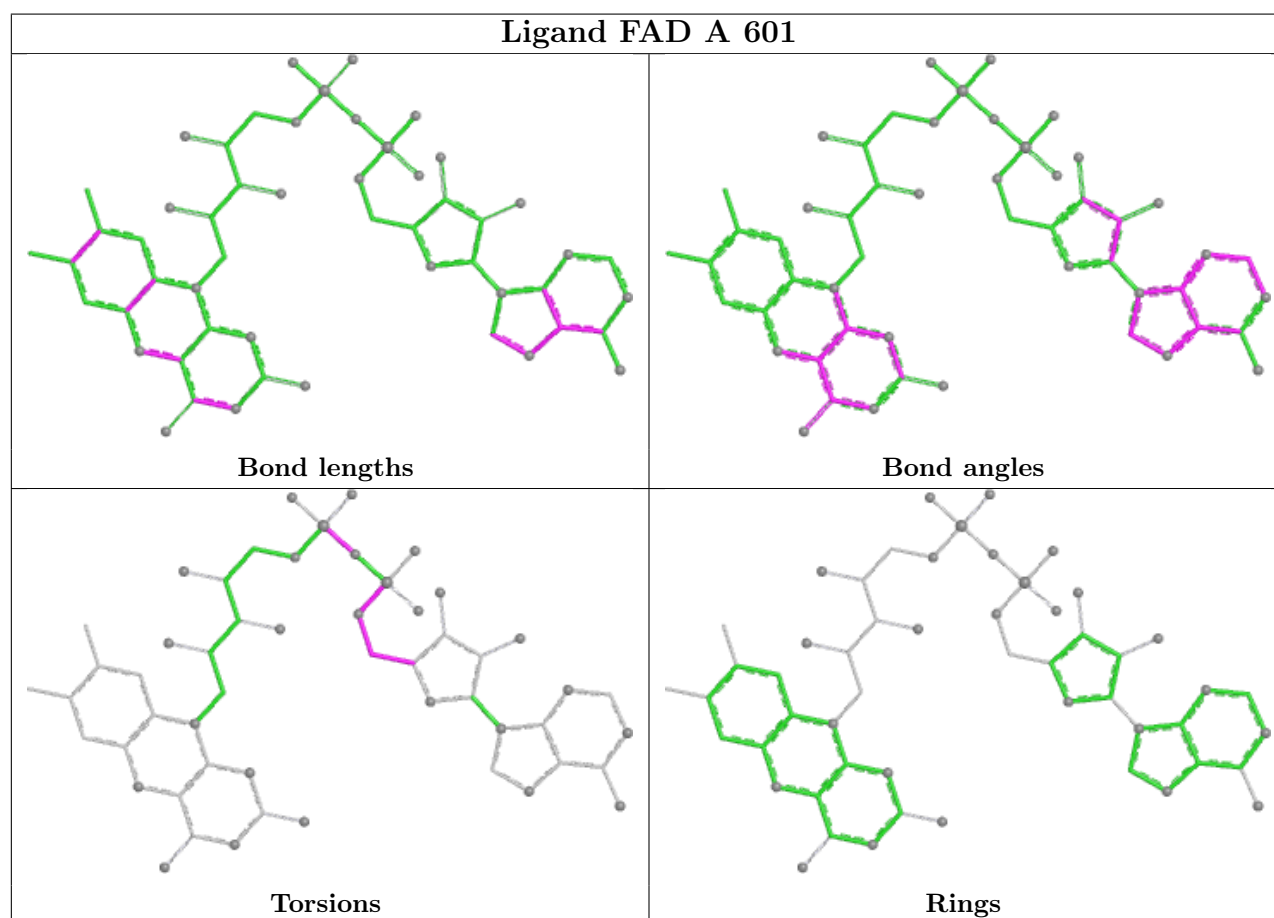
Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C5B-O5B-PA-O3P
2	B	601	FAD	C5B-O5B-PA-O3P
2	A	601	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	C3B-C4B-C5B-O5B
2	B	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	C3B-C4B-C5B-O5B
2	A	601	FAD	C4B-C5B-O5B-PA
2	B	601	FAD	C4B-C5B-O5B-PA
2	B	601	FAD	P-O3P-PA-O5B
2	A	601	FAD	C5B-O5B-PA-O1A
2	B	601	FAD	C5B-O5B-PA-O1A
2	A	601	FAD	PA-O3P-P-O2P
2	A	601	FAD	PA-O3P-P-O1P
2	B	601	FAD	PA-O3P-P-O1P
2	B	601	FAD	PA-O3P-P-O2P

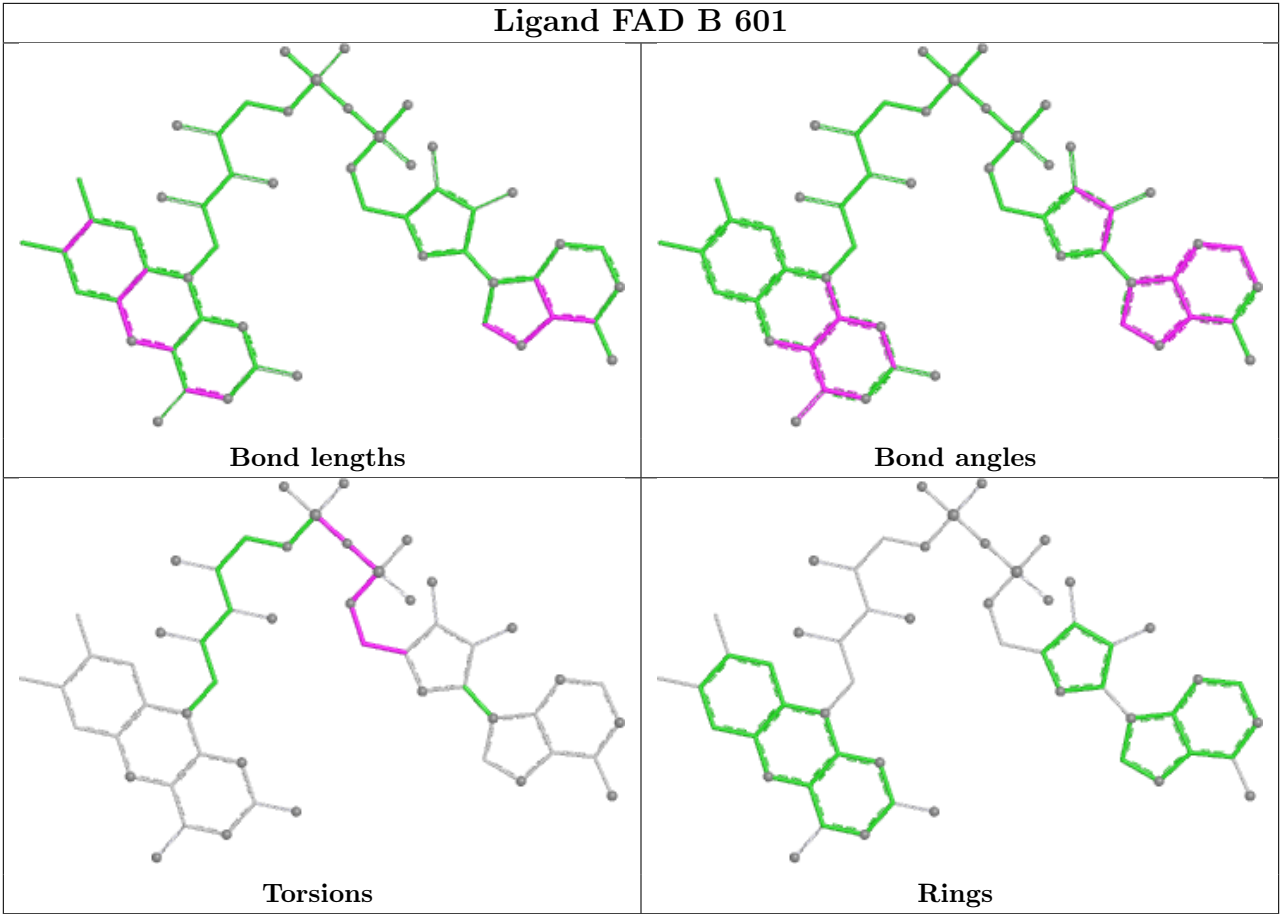
There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	11	0
2	B	601	FAD	11	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	6
1	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	179:GLY	C	180:ALA	N	1.70
1	A	69:SER	C	70:LEU	N	1.67
1	A	198:ILE	C	199:GLY	N	1.66
1	A	299:TYR	C	300:ALA	N	1.18

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	477:TRP	C	478:LEU	N	1.17
1	A	150:ASP	C	151:GLN	N	1.16
1	B	105:ALA	C	106:GLU	N	1.07
1	B	502:LEU	C	503:SER	N	0.99
1	B	354:ASP	C	355:SER	N	0.96
1	B	82:TYR	C	83:ALA	N	0.93
1	B	471:ALA	C	472:HIS	N	0.93

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	566/581 (97%)	0.82	79 (13%) 6 5	15, 31, 79, 107	0
1	B	565/581 (97%)	0.89	89 (15%) 5 4	16, 32, 77, 120	0
All	All	1131/1162 (97%)	0.85	168 (14%) 5 4	15, 32, 78, 120	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	TYR	5.6
1	A	390	ALA	5.5
1	A	282	GLU	5.2
1	B	282	GLU	5.0
1	A	392	THR	5.0
1	A	237	GLY	5.0
1	B	384	ALA	4.9
1	B	390	ALA	4.9
1	A	196	MET	4.9
1	A	263	PRO	4.8
1	A	265	ILE	4.7
1	B	198	ILE	4.5
1	B	279	GLY	4.5
1	B	388	PRO	4.4
1	A	198	ILE	4.3
1	A	236	VAL	4.3
1	A	274	ILE	4.3
1	B	200	ASP	4.2
1	B	201	SER	4.2
1	A	267	LYS	4.2
1	A	277	ILE	4.2
1	B	210	ALA	4.1
1	B	202	GLY	4.1
1	B	284	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	217	GLU	4.1
1	A	270	ALA	4.0
1	B	227	PHE	4.0
1	B	285	VAL	4.0
1	A	386	SER	4.0
1	A	394	SER	4.0
1	B	389	PRO	4.0
1	B	237	GLY	4.0
1	B	380	PRO	3.9
1	B	265	ILE	3.9
1	A	296	ASN	3.8
1	A	238	VAL	3.8
1	A	225	TRP	3.8
1	A	561	ALA	3.7
1	B	286	GLU	3.7
1	A	283	ILE	3.7
1	A	210	ALA	3.6
1	B	254	TRP	3.6
1	B	395	GLU	3.5
1	A	284	PRO	3.5
1	B	393	GLU	3.4
1	B	255	GLY	3.4
1	A	70	LEU	3.4
1	B	225	TRP	3.4
1	B	197	GLY	3.3
1	B	378	PHE	3.3
1	B	288	GLY	3.3
1	B	267	LYS	3.2
1	A	376	SER	3.2
1	A	411	ALA	3.2
1	B	401	VAL	3.1
1	B	250	TRP	3.1
1	B	217	GLU	3.1
1	A	195	GLN	3.0
1	B	391	PRO	3.0
1	A	247	TRP	3.0
1	A	212	LEU	3.0
1	B	296	ASN	3.0
1	A	397	ALA	3.0
1	A	215	LEU	2.9
1	B	398	GLU	2.9
1	B	224	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	413	ARG	2.9
1	B	263	PRO	2.9
1	B	32	SER	2.9
1	A	206	ILE	2.9
1	A	199	GLY	2.9
1	B	199	GLY	2.9
1	B	492	GLY	2.9
1	B	212	LEU	2.9
1	A	286	GLU	2.9
1	A	27	SER	2.9
1	A	194	GLY	2.9
1	A	268	GLU	2.9
1	B	238	VAL	2.9
1	A	216	CYS	2.8
1	B	382	PHE	2.8
1	A	254	TRP	2.8
1	A	200	ASP	2.8
1	A	287	VAL	2.8
1	A	7	THR	2.7
1	B	273	ILE	2.7
1	B	86	LEU	2.7
1	B	387	LEU	2.7
1	B	221	GLY	2.7
1	A	201	SER	2.7
1	B	383	GLU	2.7
1	A	278	ILE	2.6
1	A	269	GLU	2.6
1	B	215	LEU	2.6
1	B	413	ARG	2.6
1	B	216	CYS	2.6
1	A	391	PRO	2.6
1	B	6	GLU	2.5
1	A	239	ALA	2.5
1	B	195	GLN	2.5
1	B	452	ASP	2.5
1	B	359	GLU	2.5
1	A	246	PRO	2.5
1	B	204	ILE	2.5
1	B	186	GLN	2.5
1	B	287	VAL	2.5
1	B	394	SER	2.4
1	A	243	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	396	MET	2.4
1	B	397	ALA	2.4
1	B	277	ILE	2.4
1	B	361	SER	2.4
1	A	6	GLU	2.4
1	A	118	LEU	2.4
1	B	377	THR	2.4
1	A	264	GLU	2.4
1	A	135	GLY	2.4
1	A	227	PHE	2.4
1	B	77	MET	2.3
1	B	243	MET	2.3
1	B	274	ILE	2.3
1	B	249	LYS	2.3
1	A	375	LEU	2.3
1	A	378	PHE	2.3
1	B	275	HIS	2.3
1	B	392	THR	2.3
1	B	223	MET	2.3
1	B	518	LEU	2.3
1	B	407	SER	2.3
1	B	569	ARG	2.3
1	A	514	VAL	2.3
1	A	295	ILE	2.2
1	B	268	GLU	2.2
1	B	248	ASN	2.2
1	B	329	SER	2.2
1	B	87	ALA	2.2
1	A	393	GLU	2.2
1	B	252	CYS	2.2
1	A	115	TYR	2.2
1	A	400	LEU	2.2
1	B	581	SER	2.2
1	A	81	VAL	2.2
1	B	264	GLU	2.2
1	A	222	ASP	2.2
1	A	273	ILE	2.2
1	B	385	LEU	2.1
1	B	194	GLY	2.1
1	A	315	VAL	2.1
1	B	561	ALA	2.1
1	A	37	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	272	LYS	2.1
1	A	123	PHE	2.1
1	A	291	SER	2.1
1	B	247	TRP	2.1
1	A	186	GLN	2.1
1	A	38	TRP	2.1
1	B	246	PRO	2.1
1	B	151	GLN	2.1
1	B	183	LEU	2.1
1	B	303	ASN	2.1
1	A	211	ASP	2.0
1	A	409	GLU	2.0
1	B	270	ALA	2.0
1	B	408	GLU	2.0
1	A	44	GLY	2.0
1	A	202	GLY	2.0
1	A	323	GLY	2.0
1	A	221	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.

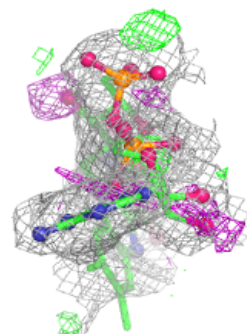
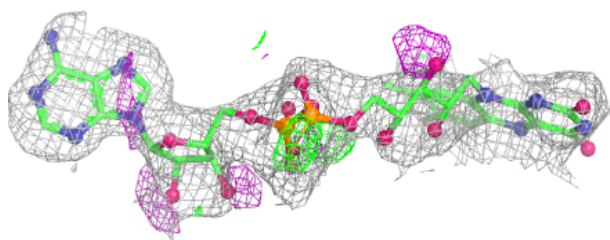
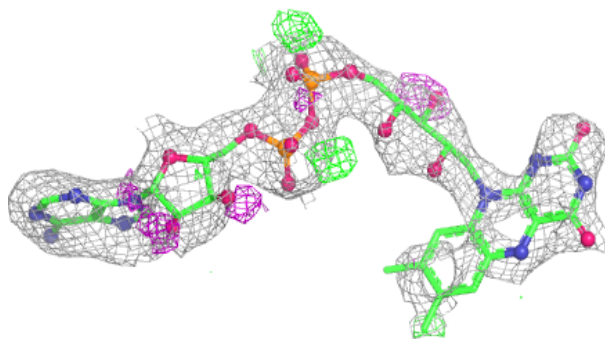
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	B	601	53/53	0.91	0.14	20,31,41,46	0
2	FAD	A	601	53/53	0.92	0.12	20,31,41,46	0

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.

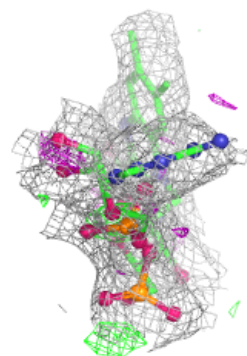
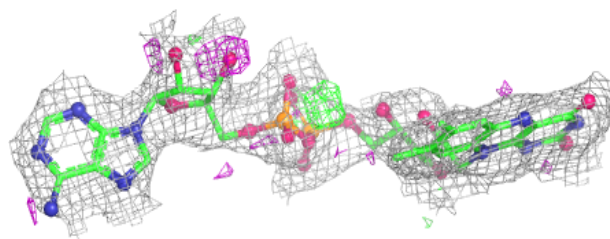
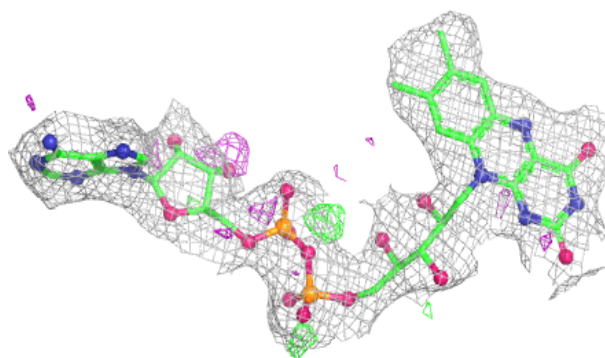
Electron density around FAD B 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FAD A 601:

$2mF_o-DF_c$ (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.