Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:14 am BST

PDB ID	:	6EM0
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 following versions of software and data (see references ⓘ) were used in the production of this report:

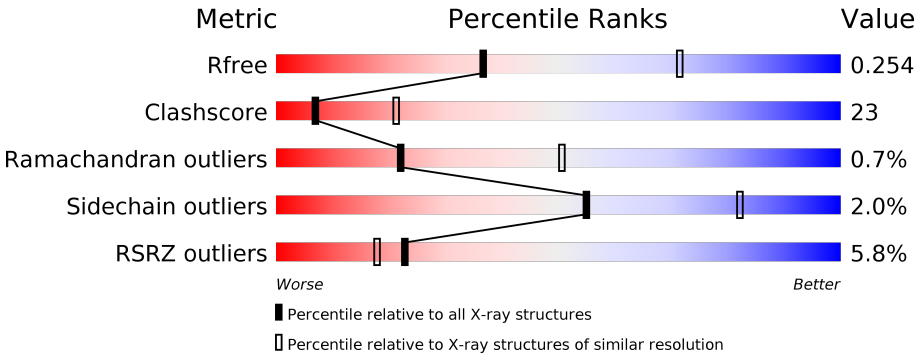
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	6% 70% 23%
1	B	581	5% 66% 26% 5%

2 Entry composition

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.

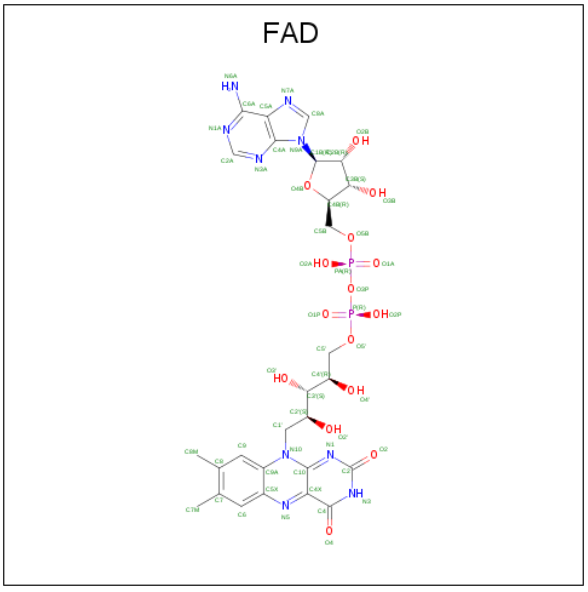
- Molecule 1 is a protein called 2-hydroxybiphenyl-3-monooxygenase.

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 (three-letter code: 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.

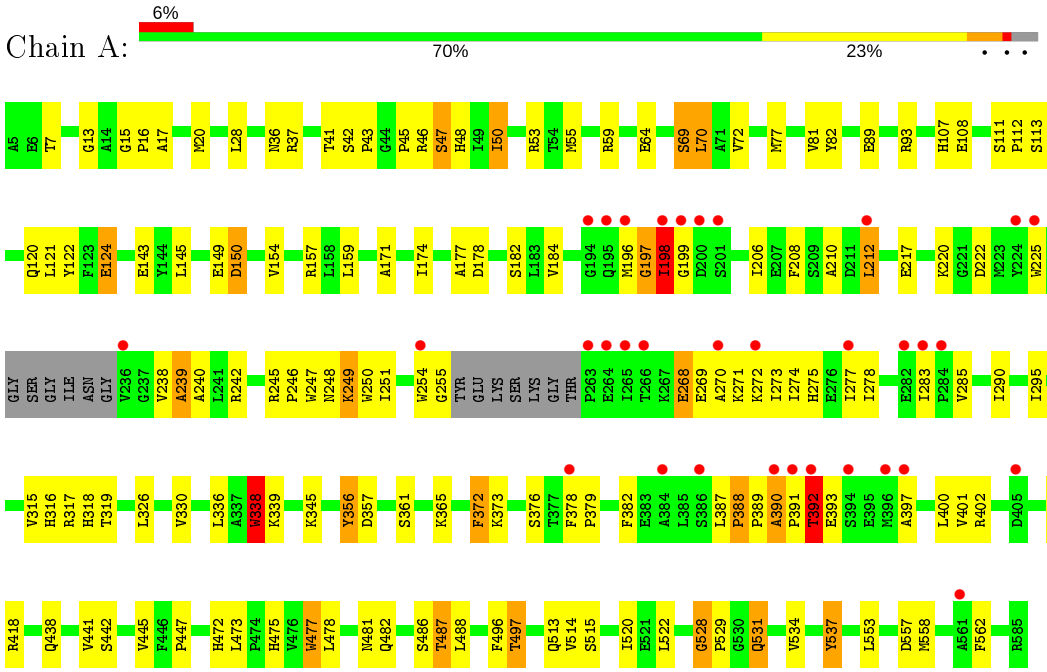
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total	O	0	0
			102	102		
3	B	74	Total	O	0	0
			74	74		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

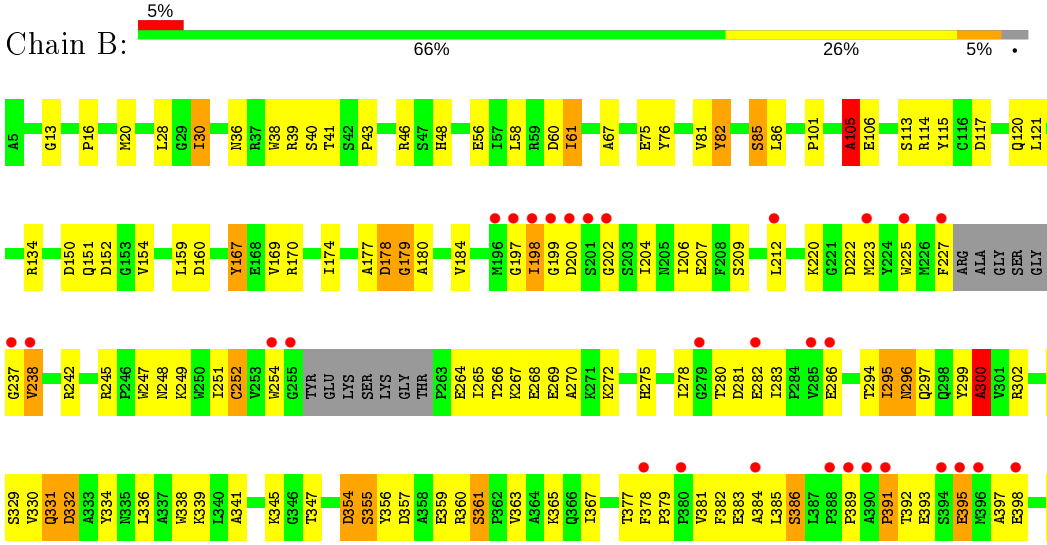
- Molecule 1: 2-hydroxybiphenyl-3-monooxygenase

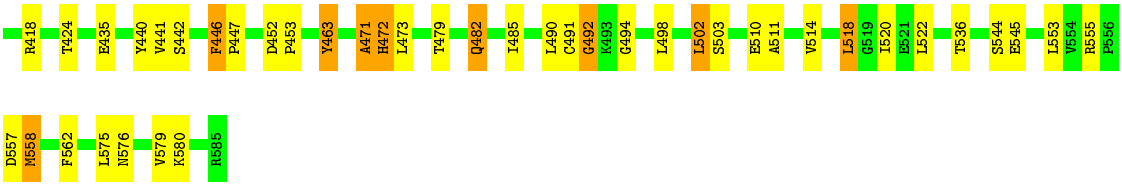
Chain A:



- Molecule 1: 2-hydroxybiphenyl-3-monooxygenase

Chain B:




R418
T424
E435
Y440
V441
S442
F446
P447
D452
P453
Y463
A471
H472
L473
T479
Q482
I485
L490
C491
G492
K493
G494
L498
L502
S503
E510
A511
V514
L518
G519
I520
E521
L522
T536
S544
E545
L553
V554
R555
P556
D557
M558
F562
L575
N576
V579
K580
R585

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.25 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.226 , 0.253 0.233 , 0.254	Depositor DCC
R_{free} test set	1716 reflections (4.94%)	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)	0.32 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.67	31/4439 (0.7%)	1.29	52/6017 (0.9%)
1	B	1.71	38/4432 (0.9%)	1.26	45/6007 (0.7%)
All	All	1.69	69/8871 (0.8%)	1.28	97/12024 (0.8%)

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 (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	528	GLY	C-O	-29.43	0.76	1.23
1	A	528	GLY	CA-C	25.65	1.92	1.51
1	A	372	PHE	CE1-CZ	25.12	1.85	1.37
1	B	472	HIS	N-CA	22.60	1.91	1.46
1	B	355	SER	N-CA	22.41	1.91	1.46
1	A	47	SER	C-O	-22.33	0.81	1.23
1	B	446	PHE	C-O	-21.85	0.81	1.23
1	B	101	PRO	CA-CB	-20.95	1.11	1.53
1	B	296	ASN	C-O	-18.49	0.88	1.23
1	A	198	ILE	C-N	18.45	1.66	1.33
1	A	149	GLU	CB-CG	-18.23	1.17	1.52
1	B	347	THR	CB-OG1	-18.20	1.06	1.43
1	B	471	ALA	C-N	-17.71	0.93	1.34
1	B	82	TYR	C-N	-17.46	0.93	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	331	GLN	CA-CB	17.42	1.92	1.53
1	B	354	ASP	C-N	-16.16	0.96	1.34
1	A	268	GLU	CB-CG	15.93	1.82	1.52
1	B	128	VAL	CA-CB	15.84	1.88	1.54
1	B	179	GLY	C-N	15.73	1.70	1.34
1	A	69	SER	C-O	-15.43	0.94	1.23
1	B	300	ALA	N-CA	15.19	1.76	1.46
1	B	502	LEU	C-N	-15.12	0.99	1.34
1	A	69	SER	C-N	14.71	1.67	1.34
1	B	389	PRO	N-CD	-14.50	1.27	1.47
1	A	299	TYR	C-O	13.88	1.49	1.23
1	A	50	ILE	CB-CG2	-13.52	1.10	1.52
1	A	531	GLN	CB-CG	13.12	1.88	1.52
1	A	50	ILE	CA-CB	13.07	1.84	1.54
1	A	513	GLN	CG-CD	-12.99	1.21	1.51
1	B	179	GLY	CA-C	-12.95	1.31	1.51
1	B	296	ASN	CA-C	12.85	1.86	1.52
1	B	502	LEU	CA-C	12.53	1.85	1.52
1	B	105	ALA	C-N	-11.74	1.07	1.34
1	B	518	LEU	CA-CB	11.46	1.80	1.53
1	A	50	ILE	CB-CG1	11.14	1.85	1.54
1	A	531	GLN	CA-CB	10.93	1.77	1.53
1	B	105	ALA	CA-C	10.81	1.81	1.52
1	B	128	VAL	CB-CG2	-10.71	1.30	1.52
1	B	30	ILE	N-CA	10.68	1.67	1.46
1	B	331	GLN	CB-CG	10.29	1.80	1.52
1	B	300	ALA	CA-CB	-10.06	1.31	1.52
1	A	47	SER	CA-C	9.75	1.78	1.52
1	B	332	ASP	CG-OD1	9.73	1.47	1.25
1	A	372	PHE	CD1-CE1	-9.15	1.21	1.39
1	A	528	GLY	C-N	9.08	1.51	1.34
1	A	47	SER	C-N	8.74	1.54	1.34
1	B	30	ILE	CA-C	-8.66	1.30	1.52
1	B	395	GLU	C-O	-8.65	1.06	1.23
1	B	300	ALA	CA-C	-8.27	1.31	1.52
1	A	239	ALA	C-O	8.06	1.38	1.23
1	A	497	THR	CA-CB	-7.80	1.33	1.53
1	A	497	THR	N-CA	-7.72	1.30	1.46
1	A	150	ASP	C-N	-7.64	1.16	1.34
1	A	477	TRP	C-N	-7.30	1.17	1.34
1	B	463	TYR	CE1-CZ	-6.86	1.29	1.38
1	A	338	TRP	C-O	-6.74	1.10	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	299	TYR	C-N	-6.73	1.18	1.34
1	B	440	TYR	CE1-CZ	-6.69	1.29	1.38
1	B	30	ILE	CA-CB	-6.54	1.39	1.54
1	A	69	SER	CA-C	6.40	1.69	1.52
1	B	61	ILE	CB-CG1	-6.17	1.36	1.54
1	B	56	GLU	CD-OE1	-5.88	1.19	1.25
1	B	356	TYR	CE1-CZ	-5.58	1.31	1.38
1	B	576	ASN	CB-CG	5.40	1.63	1.51
1	A	319	THR	CB-OG1	-5.22	1.32	1.43
1	A	250	TRP	CB-CG	-5.21	1.40	1.50
1	B	124	GLU	CD-OE1	-5.12	1.20	1.25
1	B	82	TYR	CE1-CZ	-5.09	1.31	1.38
1	A	356	TYR	CE1-CZ	-5.05	1.31	1.38

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	537	TYR	CB-CG-CD2	-26.28	105.23	121.00
1	A	537	TYR	CB-CG-CD1	26.01	136.61	121.00
1	B	300	ALA	CB-CA-C	24.24	146.46	110.10
1	A	372	PHE	CG-CD1-CE1	19.96	142.76	120.80
1	A	372	PHE	CD1-CE1-CZ	-18.39	98.03	120.10
1	B	502	LEU	O-C-N	18.11	151.67	122.70
1	B	296	ASN	O-C-N	16.63	149.31	122.70
1	B	179	GLY	CA-C-O	16.59	150.46	120.60
1	A	528	GLY	O-C-N	15.35	150.26	121.10
1	B	128	VAL	CA-CB-CG1	-13.25	91.03	110.90
1	A	50	ILE	CA-CB-CG1	-13.13	86.05	111.00
1	A	497	THR	N-CA-CB	12.98	134.97	110.30
1	B	61	ILE	CB-CG1-CD1	12.83	149.83	113.90
1	B	354	ASP	O-C-N	12.72	143.05	122.70
1	B	332	ASP	CB-CG-OD1	-12.55	107.01	118.30
1	B	502	LEU	CA-C-O	-12.18	94.52	120.10
1	B	105	ALA	CA-C-O	-12.07	94.75	120.10
1	B	30	ILE	CB-CA-C	12.06	135.73	111.60
1	B	179	GLY	O-C-N	-12.00	103.50	122.70
1	A	47	SER	CA-C-N	-11.72	91.41	117.20
1	A	69	SER	CA-C-N	-11.57	91.74	117.20
1	A	531	GLN	CA-CB-CG	-11.12	88.94	113.40
1	B	331	GLN	CA-CB-CG	-11.04	89.12	113.40
1	B	296	ASN	CA-C-N	-10.80	93.43	117.20
1	B	492	GLY	N-CA-C	10.69	139.82	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	47	SER	O-C-N	10.54	139.56	122.70
1	A	299	TYR	O-C-N	-10.53	105.85	122.70
1	A	198	ILE	O-C-N	-10.42	105.49	123.20
1	B	332	ASP	OD1-CG-OD2	-10.16	103.99	123.30
1	A	528	GLY	CA-C-N	-10.07	88.90	117.10
1	B	471	ALA	O-C-N	10.03	138.74	122.70
1	A	477	TRP	O-C-N	-9.96	106.76	122.70
1	B	354	ASP	CA-C-N	-9.71	95.83	117.20
1	A	268	GLU	N-CA-CB	9.65	127.98	110.60
1	B	446	PHE	O-C-N	9.60	139.34	121.10
1	B	61	ILE	CA-CB-CG1	9.50	129.05	111.00
1	A	299	TYR	CA-C-N	9.11	137.25	117.20
1	A	198	ILE	CA-C-O	9.08	139.17	120.10
1	B	389	PRO	CA-N-CD	9.06	124.38	111.70
1	A	149	GLU	CB-CG-CD	9.02	138.54	114.20
1	B	105	ALA	CB-CA-C	-8.82	96.87	110.10
1	B	101	PRO	CA-CB-CG	8.78	121.48	104.80
1	A	239	ALA	O-C-N	-8.36	109.33	122.70
1	A	497	THR	CA-CB-CG2	8.34	124.08	112.40
1	A	478	LEU	N-CA-CB	7.93	126.26	110.40
1	A	150	ASP	O-C-N	-7.92	110.03	122.70
1	A	338	TRP	O-C-N	7.79	135.16	122.70
1	A	513	GLN	CA-CB-CG	-7.63	96.62	113.40
1	A	268	GLU	CA-CB-CG	-7.57	96.74	113.40
1	B	471	ALA	CA-C-N	-7.53	100.64	117.20
1	A	69	SER	CB-CA-C	-7.44	95.97	110.10
1	A	338	TRP	CA-C-O	-7.42	104.51	120.10
1	B	30	ILE	CA-CB-CG1	7.30	124.86	111.00
1	B	128	VAL	CA-CB-CG2	-7.29	99.97	110.90
1	A	249	LYS	CD-CE-NZ	-7.28	94.95	111.70
1	B	446	PHE	CA-C-O	-7.24	104.90	120.10
1	A	299	TYR	CA-C-O	-7.22	104.95	120.10
1	A	149	GLU	CG-CD-OE1	-7.13	104.04	118.30
1	A	477	TRP	C-N-CA	7.06	139.35	121.70
1	B	167	TYR	CG-CD1-CE1	-7.05	115.66	121.30
1	A	392	THR	OG1-CB-CG2	7.01	126.12	110.00
1	A	528	GLY	C-N-CD	6.90	142.89	128.40
1	A	268	GLU	CB-CA-C	-6.82	96.76	110.40
1	A	41	THR	N-CA-C	-6.77	92.72	111.00
1	A	513	GLN	CG-CD-OE1	-6.73	108.14	121.60
1	A	319	THR	OG1-CB-CG2	6.71	125.44	110.00
1	B	296	ASN	C-N-CA	-6.68	105.01	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	197	GLY	N-CA-C	-6.67	96.43	113.10
1	A	531	GLN	CB-CA-C	-6.64	97.12	110.40
1	A	149	GLU	CG-CD-OE2	6.61	131.52	118.30
1	B	518	LEU	CA-CB-CG	-6.56	100.22	115.30
1	A	198	ILE	CA-C-N	-6.29	103.61	116.20
1	B	576	ASN	CA-CB-CG	-6.24	99.67	113.40
1	A	497	THR	CA-C-N	6.19	130.82	117.20
1	A	497	THR	CA-C-O	-6.07	107.35	120.10
1	B	61	ILE	CG1-CB-CG2	-6.04	98.11	111.40
1	A	50	ILE	CB-CA-C	-6.03	99.53	111.60
1	A	50	ILE	N-CA-CB	6.01	124.62	110.80
1	B	179	GLY	CA-C-N	-5.98	104.05	117.20
1	A	69	SER	N-CA-C	5.88	126.88	111.00
1	B	178	ASP	CB-CG-OD2	-5.79	113.08	118.30
1	B	105	ALA	O-C-N	5.78	131.95	122.70
1	A	47	SER	C-N-CA	-5.67	107.53	121.70
1	A	239	ALA	CA-C-O	5.66	131.98	120.10
1	B	354	ASP	C-N-CA	-5.58	107.74	121.70
1	B	41	THR	N-CA-C	-5.39	96.45	111.00
1	A	388	PRO	C-N-CD	5.35	139.63	128.40
1	A	198	ILE	N-CA-C	-5.30	96.69	111.00
1	B	85	SER	N-CA-C	-5.28	96.75	111.00
1	B	85	SER	CB-CA-C	5.28	120.12	110.10
1	B	332	ASP	CA-CB-CG	5.27	124.99	113.40
1	A	413	ARG	C-N-CA	-5.21	108.67	121.70
1	B	81	VAL	CB-CA-C	-5.21	101.51	111.40
1	B	498	LEU	CA-CB-CG	5.20	127.27	115.30
1	B	518	LEU	CB-CG-CD2	-5.18	102.20	111.00
1	B	389	PRO	N-CA-CB	-5.16	96.93	102.60
1	B	518	LEU	N-CA-CB	5.10	120.61	110.40

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

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Mol	Chain	Res	Type	Group
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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4344	0	4292	194	0
1	B	4337	0	4281	204	0
2	A	53	0	31	10	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	8635	401	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 23.

All (401) 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:CA	1:B:518:LEU:CB	1.80	1.59
1:B:331:GLN:CB	1:B:331:GLN:CG	1.80	1.58
1:A:372:PHE:CE1	1:A:372:PHE:CZ	1.85	1.57
1:A:50:ILE:CB	1:A:50:ILE:CG1	1.85	1.55
1:B:30:ILE:N	1:B:30:ILE:CA	1.67	1.55
1:A:268:GLU:CB	1:A:268:GLU:CG	1.82	1.53
1:A:50:ILE:CA	1:A:50:ILE:CB	1.84	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:VAL:CB	1:B:128:VAL:CA	1.88	1.52
1:A:47:SER:C	1:A:47:SER:CA	1.78	1.51
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:105:ALA:C	1:B:105:ALA:CA	1.81	1.47
1:A:69:SER:C	1:A:70:LEU:N	1.67	1.46
1:B:179:GLY:C	1:B:180:ALA:N	1.70	1.45
1:B:331:GLN:CB	1:B:331:GLN:CA	1.92	1.44
1:B:502:LEU:C	1:B:502:LEU:CA	1.85	1.44
1:B:296:ASN:C	1:B:296:ASN:CA	1.86	1.41
1:A:528:GLY:C	1:A:528:GLY:CA	1.92	1.38
1:B:355:SER:N	1:B:355:SER:CA	1.91	1.32
1:B:472:HIS:N	1:B:472:HIS:CA	1.91	1.32
1:B:223:MET:HE1	1:B:225:TRP:CZ2	1.73	1.22
1:B:446:PHE:O	1:B:446:PHE:CA	1.90	1.18
1:B:223:MET:HE3	1:B:225:TRP:CE2	1.80	1.17
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	1.15
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:82:TYR:HE1	1:A:225:TRP:CE3	1.66	1.13
1:B:223:MET:HE3	1:B:225:TRP:NE1	1.63	1.12
1:A:82:TYR:CE1	1:A:225:TRP:HE3	1.71	1.09
1:A:389:PRO:C	1:A:391:PRO:HD2	1.72	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: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:81:VAL:HG22	1:A:93:ARG:HD3	1.37	1.04
1:B:446:PHE:C	1:B:446:PHE:O	0.81	1.01
1:A:372:PHE:CD1	1:A:372:PHE:CZ	2.34	1.00
1:A:47:SER:C	1:A:47:SER:O	0.80	0.99
1:B:252:CYS:HB3	1:B:254:TRP:HZ3	1.22	0.99
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:528:GLY:C	1:A:528:GLY:O	0.76	0.95
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:223:MET:HE1	1:B:225:TRP:HZ2	1.32	0.91
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:354:ASP:C	1:B:355:SER:CA	2.39	0.90
1:B:266:THR:CG2	1:B:270:ALA:HB2	2.02	0.90
1:B:223:MET:HE1	1:B:225:TRP:CE2	2.03	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:212:LEU:HD21	1:A:278:ILE:HD13	1.56	0.87
1:A:77:MET:HB2	1:A:222:ASP:HB2	1.53	0.87
1:A:50:ILE:CA	1:A:50:ILE:CG1	2.52	0.87
1:A:50:ILE:CG2	1:A:50:ILE:CA	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:471:ALA:C	1:B:472:HIS:CA	2.44	0.86
1:B:206:ILE:HD12	1:B:254:TRP:HH2	1.39	0.85
1:A:50:ILE:CG2	1:A:50:ILE:CG1	2.51	0.85
1:A:212:LEU:CD1	1:A:283:ILE:HG21	2.07	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:CA	1:A:268:GLU:CG	2.56	0.83
1:A:531:GLN:C	1:A:531:GLN:CB	2.47	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:CG	1:A:531:GLN:CA	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: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:511:ALA:HB1	1:B:522:LEU:HD22	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:105:ALA:C	1:B:105:ALA:CB	2.48	0.80
1:B:39:ARG:HH11	1:B:39:ARG:HG2	1.46	0.80
1:B:518:LEU:CA	1:B:518:LEU:CG	2.60	0.80
1:B:300:ALA:CB	1:B:300:ALA:N	2.45	0.80
1:A:220:LYS:HG2	1:A:247:TRP:HZ2	1.47	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:502:LEU:CA	1:B:503:SER:N	2.42	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: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: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:A:113:SER:C	1:A:114:ARG:HG2	2.05	0.76
1:B:492:GLY:O	3:B:701:HOH:O	2.02	0.76
1:B:382:PHE:O	1:B:383:GLU:C	2.20	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: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:O	1:B:502:LEU:CA	2.34	0.74
1:B:46:ARG:CD	2:B:601:FAD:C7	2.62	0.74
1:A:47:SER:CA	1:A:47:SER:O	2.36	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:B:223:MET:CE	1:B:225:TRP:HE1	2.01	0.73
1:B:30:ILE:N	1:B:30:ILE:CB	2.48	0.73
1:A:357:ASP:O	1:A:361:SER:HB2	1.89	0.73
1:A:389:PRO:C	1:A:391:PRO:CD	2.56	0.72
1:B:331:GLN:CB	1:B:331:GLN:CD	2.57	0.72
1:A:274:ILE:C	1:A:277:ILE:HG22	2.09	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:CB	1:A:50:ILE:C	2.58	0.72
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:47:SER:N	1:A:47:SER:C	2.43	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: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:518:LEU:C	1:B:518:LEU:CB	2.59	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: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:A:69:SER:C	1:A:70:LEU:CA	2.61	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:46:ARG:HD3	2:B:601:FAD:C6	2.24	0.66
1:A:515:SER:HB2	1:A:520:ILE:O	1.96	0.66
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:300:ALA:N	1:B:300:ALA:C	2.45	0.65
1:B:13:GLY:HA2	2:B:601:FAD:O4B	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:SER:O	1:B:359:GLU:CB	2.46	0.63
1:B:58:LEU:HD13	1:B:67:ALA:HB2	1.80	0.63
1:A:89:GLU:OE1	1:A:400:LEU:CD2	2.47	0.63
1:A:278:ILE:HG21	1:A:283:ILE:HD12	1.80	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:382:PHE:C	1:B:384:ALA:N	2.50	0.62
1:A:121:LEU:HD23	1:A:122:TYR:CE1	2.35	0.62
1:A:50:ILE:CD1	1:A:50:ILE:HG23	2.30	0.62
1:A:157:ARG:HH11	1:A:157:ARG:HG3	1.65	0.61
1:B:331:GLN:CB	1:B:331:GLN:C	2.68	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: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:HG	1:B:336:LEU:O	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:HG12	1:A:50:ILE:N	2.15	0.60
1:A:208:PHE:HD1	1:A:285:VAL:HG13	1.66	0.60
1:A:208:PHE:CD1	1:A:285:VAL:HG13	2.37	0.60
1:A:50:ILE:CD1	1:A:50:ILE:CB	2.76	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:O	1:A:196:MET:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:296:ASN:C	1:B:296:ASN:CB	2.71	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:557:ASP:O	1:A:558:MET:HB2	2.02	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:B:473:LEU:HD23	1:B:558:MET:CE	2.35	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:A:388:PRO:HG2	1:A:391:PRO:CD	2.34	0.56
1:A:59:ARG:HG3	1:A:64:GLU:OE1	2.05	0.56
1:B:386:SER:CB	1:B:402:ARG:HH21	2.18	0.56
1:B:178:ASP:OD2	1:B:184:VAL:HG23	2.05	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:B:266:THR:HG23	1:B:269:GLU:HG3	1.86	0.56
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: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: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:O	1:B:238:VAL:HG12	2.07	0.54
1:B:30:ILE:N	1:B:30:ILE:C	2.46	0.54
1:A:531:GLN:N	1:A:531:GLN:CB	2.64	0.54
1:B:150:ASP:OD1	1:B:152:ASP:N	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:PHE:CB	1:B:446:PHE:O	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:O	1:B:169:VAL:HG13	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:296:ASN:C	1:B:296:ASN:N	2.57	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: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:B:46:ARG:CD	2:B:601:FAD:C8	2.87	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
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:487:THR:C	2.48	0.52
1:A:486:SER:O	1:A:488:LEU:N	2.43	0.52
1:B:225:TRP:HH2	1:B:378:PHE:CZ	2.27	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:39:ARG:NH1	1:B:39:ARG:HG2	2.19	0.52
1:B:46:ARG:HB2	1:B:120:GLN:OE1	2.10	0.52
1:B:76:TYR:CD1	1:B:76:TYR:N	2.78	0.52
1:A:528:GLY:C	1:A:534:VAL:HG13	2.31	0.51
1:A:53:ARG:NH1	1:A:438:GLN:OE1	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:VAL:N	1:B:128:VAL:CB	2.64	0.51
1:B:294:THR:C	1:B:295:ILE:HG13	2.31	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:B:199:GLY:O	1:B:200:ASP:C	2.48	0.51
1:A:13:GLY:HA2	2:A:601:FAD:O4B	2.11	0.51
1:A:17:ALA:O	1:A:311:MET:HE1	2.11	0.50
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:178:ASP:OD2	1:A:184:VAL:HG23	2.11	0.50
1:A:122:TYR:HE2	1:A:245:ARG:NH1	1.99	0.50
1:B:76:TYR:HD1	1:B:76:TYR:N	2.10	0.50
1:A:336:LEU:O	1:A:336:LEU:HG	2.10	0.50
1:B:325:GLY:O	1:B:329:SER:OG	2.24	0.50
1:A:177:ALA:HB2	1:A:311:MET:HE3	1.93	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:518:LEU:HB2	1:B:520:ILE:HG22	1.93	0.49
1:A:157:ARG:NH1	1:A:157:ARG:HG3	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
1:B:113:SER:O	1:B:114:ARG:NH1	2.46	0.49
1:B:39:ARG:NH1	1:B:39:ARG:CG	2.72	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:178:ASP:N	1:A:178:ASP:OD1	2.39	0.49
1:A:397:ALA:O	1:A:401:VAL:HG23	2.13	0.49
1:A:50:ILE:CG2	1:A:50:ILE:CD1	2.89	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:HG13	1:A:238:VAL:O	2.14	0.48
1:B:86:LEU:HD21	1:B:212:LEU:HD13	1.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:SER:HB3	1:A:120:GLN:HG3	1.96	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:47:SER:CB	1:A:47:SER:C	2.74	0.47
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: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:242:ARG:HB3	1:A:251:ILE:HG22	1.97	0.46
1:A:326:LEU:C	1:A:326:LEU:HD23	2.36	0.46
1:A:89:GLU:OE1	1:A:400:LEU:HD21	2.14	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:378:PHE:C	1:A:378:PHE:CD1	2.89	0.46
1:A:42:SER:CB	1:A:124:GLU:OE1	2.62	0.46
1:A:178:ASP:C	2:A:601:FAD:H52A	2.36	0.46
1:B:384:ALA:C	1:B:386:SER:H	2.18	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
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:B:485:ILE:HD13	1:B:490:LEU:CD1	2.46	0.45
1:A:17:ALA:HB1	1:A:311:MET:CE	2.46	0.45
1:B:16:PRO:HD2	2:B:601:FAD:O2P	2.16	0.45
1:A:242:ARG:HB3	1:A:251:ILE:CG2	2.47	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: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:B:223:MET:HE3	1:B:225:TRP:CD1	2.45	0.44
1:B:502:LEU:C	1:B:502:LEU:CB	2.76	0.44
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:A:373:LYS:O	1:A:376:SER:OG	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:GLY:C	1:B:198:ILE:O	2.57	0.43
1:B:220:LYS:HG2	1:B:247:TRP:CZ2	2.54	0.43
1:B:297:GLN:HG2	1:B:318:HIS:HA	2.01	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:113:SER:C	1:A:114:ARG:CG	2.85	0.42
1:A:315:VAL:HG23	1:A:316:HIS:CD2	2.54	0.42
1:A:69:SER:N	1:A:70:LEU:N	2.67	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:225:TRP:HH2	1:B:378:PHE:CE1	2.38	0.41
1:B:13:GLY:HA2	2:B:601:FAD:C1B	2.49	0.41
1:A:295:ILE:CD1	1:A:318:HIS:N	2.79	0.41
1:B:296:ASN:CA	1:B:296:ASN:O	2.39	0.41
1:A:378:PHE:N	1:A:379:PRO:HD2	2.35	0.41
1:A:311:MET:HB3	1:A:356:TYR:OH	2.20	0.41
1:B:128:VAL:C	1:B:128:VAL:HG12	2.40	0.41
1:B:60:ASP:OD1	1:B:492:GLY:O	2.38	0.41
1:B:491:CYS:HB2	1:B:558:MET:HE3	2.02	0.41
1:B:223:MET:SD	1:B:225:TRP:NE1	2.93	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

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%)	17 44
1	B	559/581 (96%)	507 (91%)	49 (9%)	3 (0%)	29 58
All	All	1119/1162 (96%)	1010 (90%)	101 (9%)	8 (1%)	22 50

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 (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	452/462 (98%)	442 (98%)	10 (2%)	52 80
1	B	451/462 (98%)	443 (98%)	8 (2%)	59 84
All	All	903/924 (98%)	885 (98%)	18 (2%)	55 82

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LEU
1	A	124	GLU
1	A	198	ILE
1	A	212	LEU
1	A	275	HIS
1	A	311	MET

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Mol	Chain	Res	Type
1	A	317	ARG
1	A	392	THR
1	A	497	THR
1	A	537	TYR
1	B	248	ASN
1	B	252	CYS
1	B	295	ILE
1	B	361	SER
1	B	386	SER
1	B	463	TYR
1	B	482	GLN
1	B	558	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	195	GLN
1	B	52	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	A	601	-	51,58,58	1.87	6 (11%)	60,89,89	1.97	13 (21%)
2	FAD	B	601	-	51,58,58	1.86	6 (11%)	60,89,89	1.97	13 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	601	-	-	7/30/50/50	0/6/6/6
2	FAD	B	601	-	-	9/30/50/50	0/6/6/6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C4X-C10	9.70	1.48	1.38
2	A	601	FAD	C4X-C10	9.67	1.48	1.38
2	B	601	FAD	C4-C4X	4.27	1.48	1.41
2	A	601	FAD	C4-C4X	4.25	1.48	1.41
2	A	601	FAD	C9A-C5X	3.55	1.49	1.42
2	B	601	FAD	C9A-C5X	3.51	1.49	1.42
2	B	601	FAD	C8-C7	3.30	1.49	1.40
2	A	601	FAD	C8-C7	3.29	1.49	1.40
2	B	601	FAD	C5A-C4A	2.51	1.47	1.40
2	A	601	FAD	C5A-C4A	2.51	1.47	1.40
2	B	601	FAD	C9A-N10	2.09	1.41	1.38
2	A	601	FAD	C9A-N10	2.07	1.41	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	FAD	C4-N3-C2	8.48	122.30	115.14
2	A	601	FAD	C4-N3-C2	8.40	122.24	115.14
2	A	601	FAD	C4-C4X-C10	-5.06	116.60	119.95
2	B	601	FAD	C4-C4X-C10	-5.01	116.63	119.95
2	B	601	FAD	C4X-N5-C5X	3.98	120.75	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	FAD	C4X-N5-C5X	3.96	120.73	116.77
2	B	601	FAD	C4X-C4-N3	-3.66	118.43	123.43
2	A	601	FAD	C4X-C4-N3	-3.63	118.47	123.43
2	B	601	FAD	P-O3P-PA	-3.60	120.49	132.83
2	A	601	FAD	P-O3P-PA	-3.58	120.54	132.83
2	A	601	FAD	C3B-C2B-C1B	3.55	106.32	100.98
2	B	601	FAD	C3B-C2B-C1B	3.51	106.27	100.98
2	B	601	FAD	C1'-N10-C9A	3.19	120.80	118.29
2	B	601	FAD	N3A-C2A-N1A	-3.17	123.72	128.68
2	A	601	FAD	N3A-C2A-N1A	-3.17	123.73	128.68
2	A	601	FAD	C1'-N10-C9A	3.13	120.76	118.29
2	B	601	FAD	C4-C4X-N5	3.10	122.14	118.60
2	A	601	FAD	C4-C4X-N5	3.08	122.12	118.60
2	A	601	FAD	C4A-C5A-N7A	-2.69	106.60	109.40
2	B	601	FAD	C9A-N10-C10	-2.68	118.39	121.91
2	A	601	FAD	C1'-N10-C10	2.68	120.81	118.41
2	B	601	FAD	C1'-N10-C10	2.67	120.80	118.41
2	B	601	FAD	C4A-C5A-N7A	-2.67	106.62	109.40
2	A	601	FAD	C9A-N10-C10	-2.65	118.43	121.91
2	B	601	FAD	C5X-C9A-N10	2.49	119.52	117.72
2	A	601	FAD	C5X-C9A-N10	2.46	119.50	117.72

There are no chirality outliers.

All (16) torsion outliers are listed below:

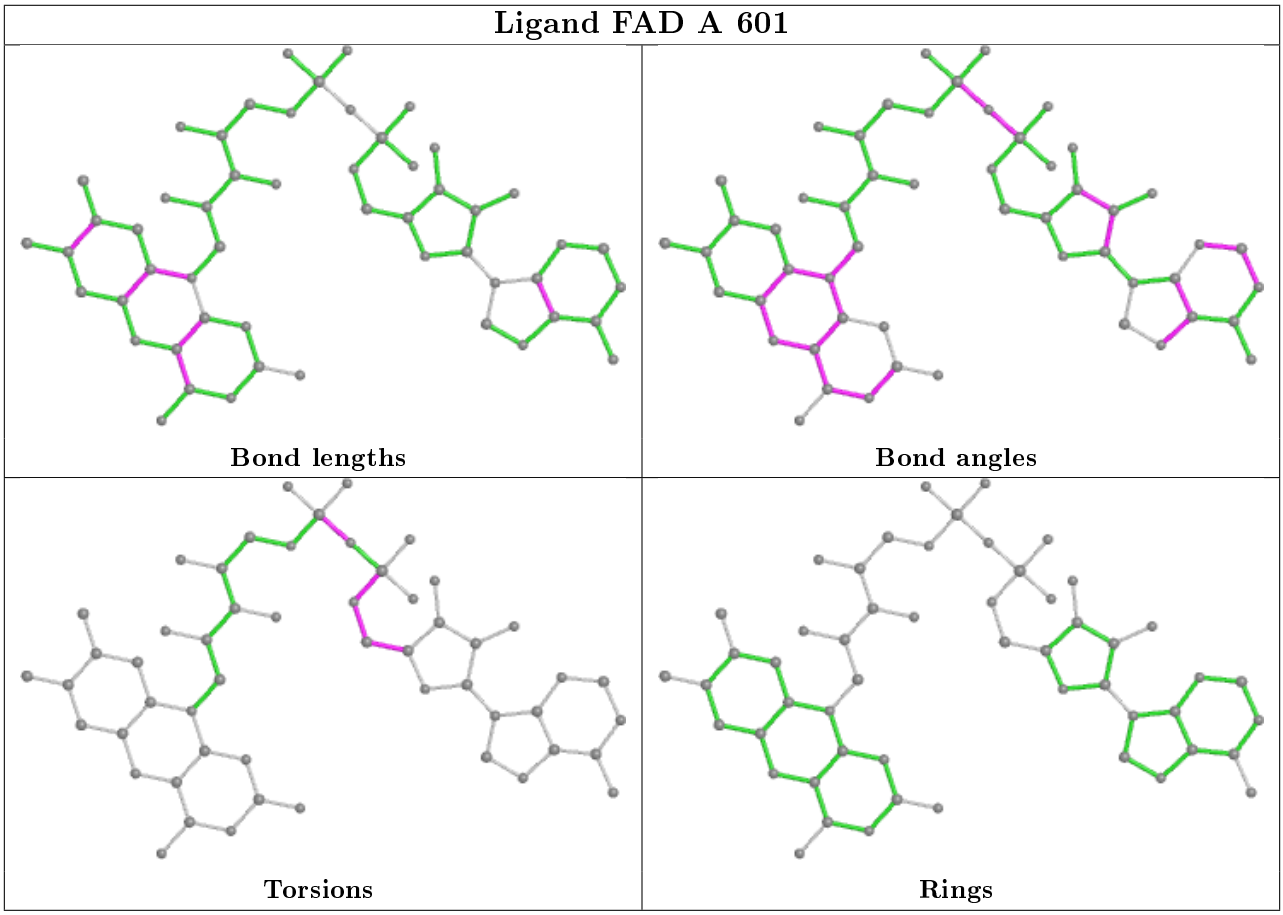
Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C5B-O5B-PA-O3P
2	B	601	FAD	C5B-O5B-PA-O3P
2	A	601	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	C3B-C4B-C5B-O5B
2	B	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	C3B-C4B-C5B-O5B
2	A	601	FAD	C4B-C5B-O5B-PA
2	B	601	FAD	C4B-C5B-O5B-PA
2	B	601	FAD	P-O3P-PA-O5B
2	A	601	FAD	C5B-O5B-PA-O1A
2	B	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
2	B	601	FAD	O4'-C4'-C5'-O5'

There are no ring outliers.

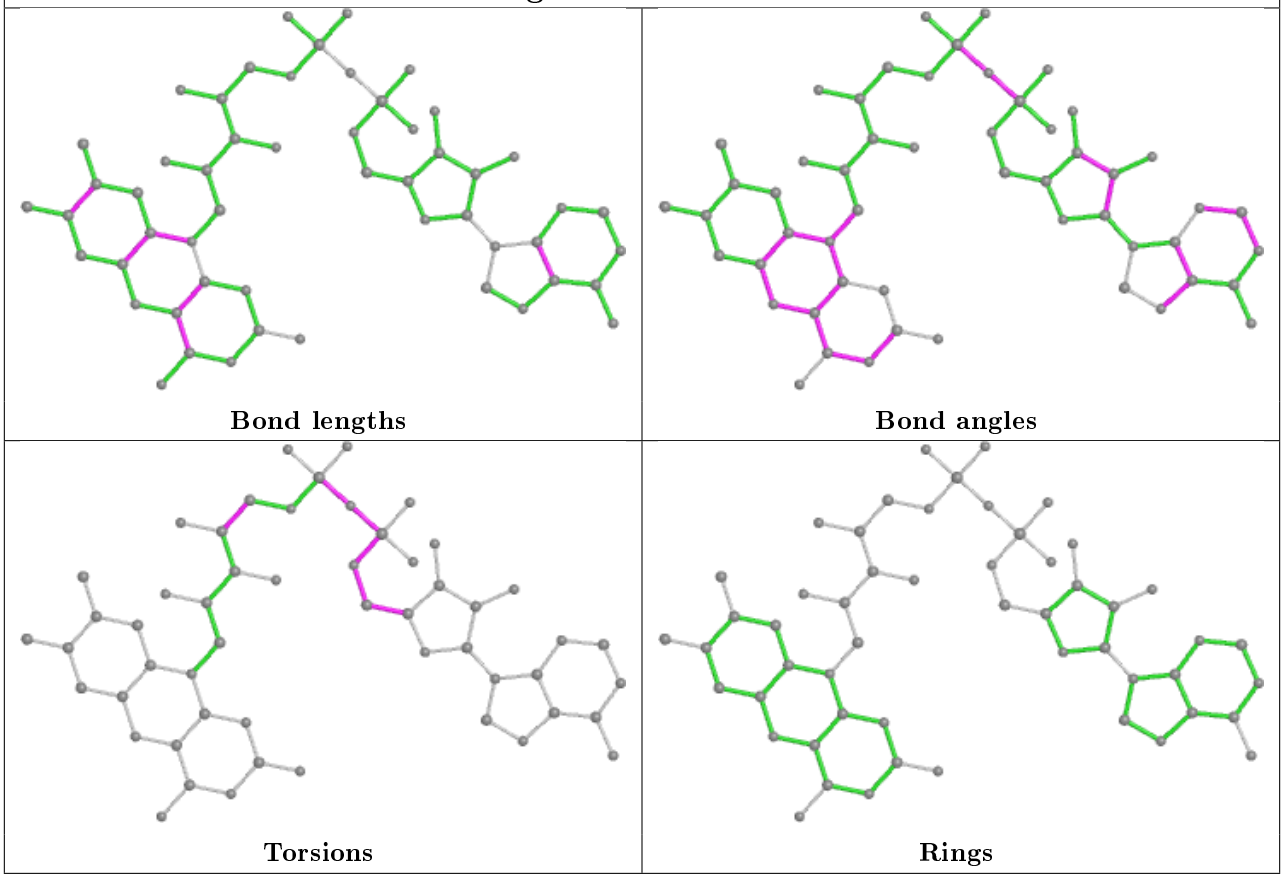
2 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	10	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 then 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.



Ligand FAD B 601



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
1	A	477:TRP	C	478:LEU	N	1.17

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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, 95^{th} 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%)	0.24	35 (6%)	20	15	15, 31, 79, 107	0
1	B	565/581 (97%)	0.23	31 (5%)	25	19	16, 32, 77, 120	0
All	All	1131/1162 (97%)	0.24	66 (5%)	23	18	15, 32, 78, 120	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	388	PRO	5.6
1	B	237	GLY	5.5
1	A	263	PRO	5.4
1	B	198	ILE	5.1
1	B	396	MET	4.9
1	B	202	GLY	4.9
1	A	236	VAL	4.6
1	B	238	VAL	4.2
1	A	390	ALA	4.2
1	A	254	TRP	4.2
1	B	201	SER	4.1
1	B	282	GLU	4.1
1	B	390	ALA	4.1
1	A	196	MET	4.0
1	B	384	ALA	4.0
1	B	286	GLU	4.0
1	B	200	ASP	3.9
1	A	195	GLN	3.9
1	B	227	PHE	3.8
1	A	199	GLY	3.8
1	B	197	GLY	3.7
1	B	389	PRO	3.7
1	A	224	TYR	3.6
1	B	398	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	386	SER	3.5
1	A	394	SER	3.4
1	A	198	ILE	3.3
1	B	212	LEU	3.2
1	A	200	ASP	3.2
1	A	392	THR	3.2
1	A	391	PRO	3.1
1	B	380	PRO	3.1
1	A	282	GLU	3.1
1	A	265	ILE	3.0
1	A	270	ALA	3.0
1	B	378	PHE	3.0
1	B	254	TRP	3.0
1	B	285	VAL	3.0
1	B	196	MET	2.9
1	A	378	PHE	2.8
1	B	199	GLY	2.8
1	B	225	TRP	2.8
1	A	272	LYS	2.7
1	A	277	ILE	2.7
1	A	284	PRO	2.6
1	A	194	GLY	2.6
1	B	279	GLY	2.5
1	A	384	ALA	2.5
1	B	395	GLU	2.5
1	A	283	ILE	2.5
1	B	394	SER	2.4
1	A	405	ASP	2.4
1	A	561	ALA	2.4
1	B	255	GLY	2.3
1	A	264	GLU	2.3
1	B	223	MET	2.3
1	A	396	MET	2.3
1	A	413	ARG	2.3
1	A	212	LEU	2.2
1	B	391	PRO	2.1
1	A	266	THR	2.1
1	A	201	SER	2.1
1	A	225	TRP	2.1
1	A	397	ALA	2.1
1	A	227	PHE	2.1
1	B	407	SER	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 carbohydrates in this entry.

6.4 Ligands (i)

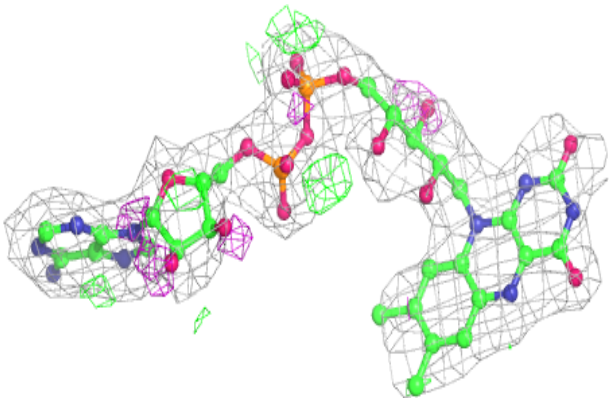
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

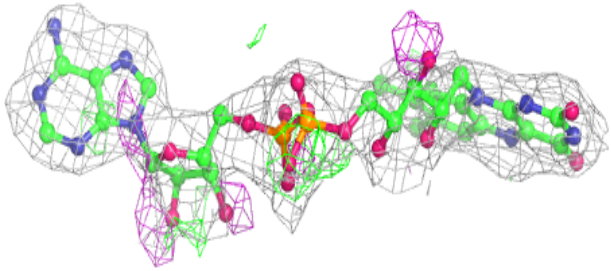
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	B	601	53/53	0.93	0.21	20,31,41,46	0
2	FAD	A	601	53/53	0.94	0.18	20,31,41,46	0

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:

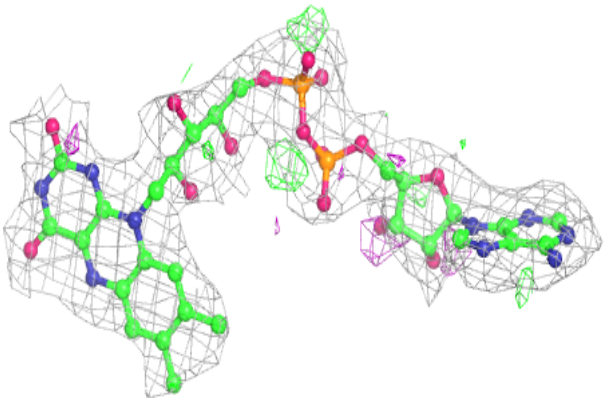
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

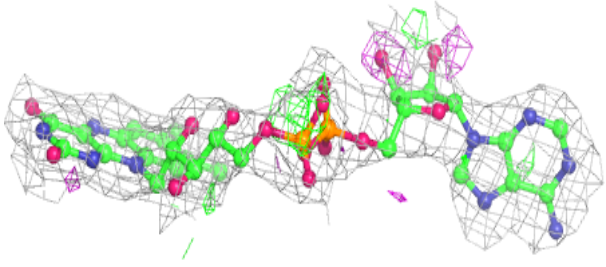


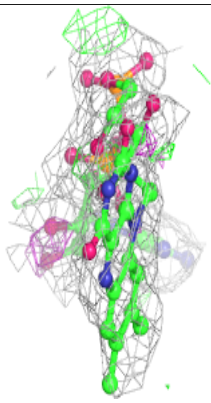


Electron density around FAD A 601:

$2mF_o$-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.