



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 07:50 pm BST

PDB ID : 3AYL
Title : X-ray crystal structures of L-phenylalanine oxidase (deaminating and decarboxylating) from *Pseudomonas* sp. P501. Structures of the enzyme-ligand complex and catalytic mechanism
Authors : Suzuki, H.
Deposited on : 2011-05-07
Resolution : 1.25 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

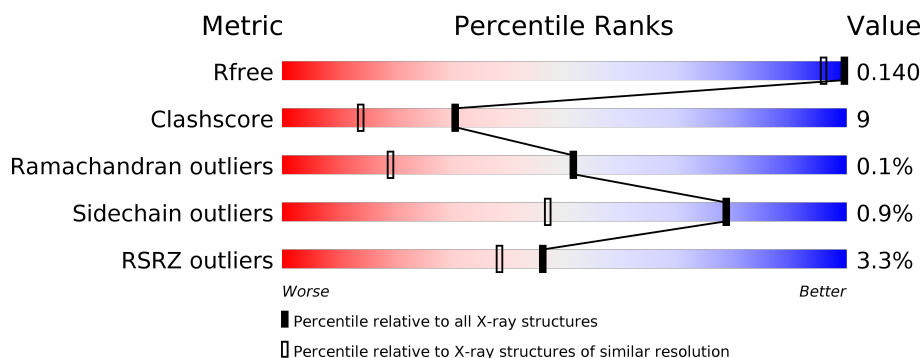
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.25 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	1023 (1.28-1.24)
Clashscore	141614	1060 (1.28-1.24)
Ramachandran outliers	138981	1029 (1.28-1.24)
Sidechain outliers	138945	1028 (1.28-1.24)
RSRZ outliers	127900	1004 (1.28-1.24)

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 $\leq 5\%$. 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	721	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>• • 5%</div> </div> </div>
1	B	721	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>• • 5%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	3001	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12791 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.

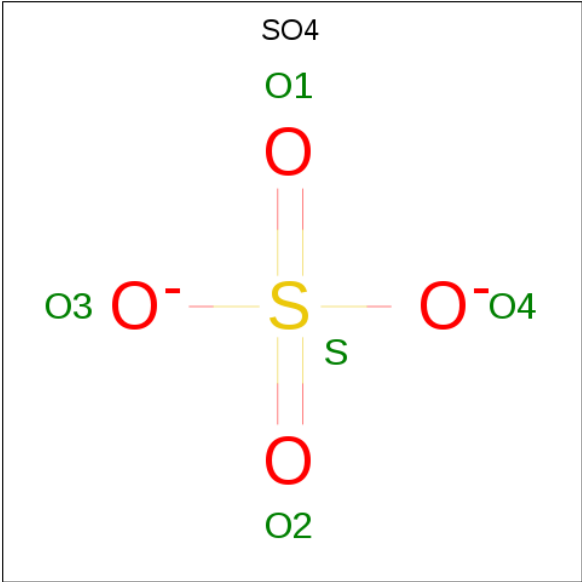
- Molecule 1 is a protein called Pro-enzyme of L-phenylalanine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	684	Total	C	N	O	S	0	0	0
			5212	3326	902	973	11			
1	B	684	Total	C	N	O	S	0	0	0
			5212	3326	902	973	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	714	LEU	-	EXPRESSION TAG	UNP Q5W9R9
A	715	GLU	-	EXPRESSION TAG	UNP Q5W9R9
A	716	HIS	-	EXPRESSION TAG	UNP Q5W9R9
A	717	HIS	-	EXPRESSION TAG	UNP Q5W9R9
A	718	HIS	-	EXPRESSION TAG	UNP Q5W9R9
A	719	HIS	-	EXPRESSION TAG	UNP Q5W9R9
A	720	HIS	-	EXPRESSION TAG	UNP Q5W9R9
A	721	HIS	-	EXPRESSION TAG	UNP Q5W9R9
B	714	LEU	-	EXPRESSION TAG	UNP Q5W9R9
B	715	GLU	-	EXPRESSION TAG	UNP Q5W9R9
B	716	HIS	-	EXPRESSION TAG	UNP Q5W9R9
B	717	HIS	-	EXPRESSION TAG	UNP Q5W9R9
B	718	HIS	-	EXPRESSION TAG	UNP Q5W9R9
B	719	HIS	-	EXPRESSION TAG	UNP Q5W9R9
B	720	HIS	-	EXPRESSION TAG	UNP Q5W9R9
B	721	HIS	-	EXPRESSION TAG	UNP Q5W9R9

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



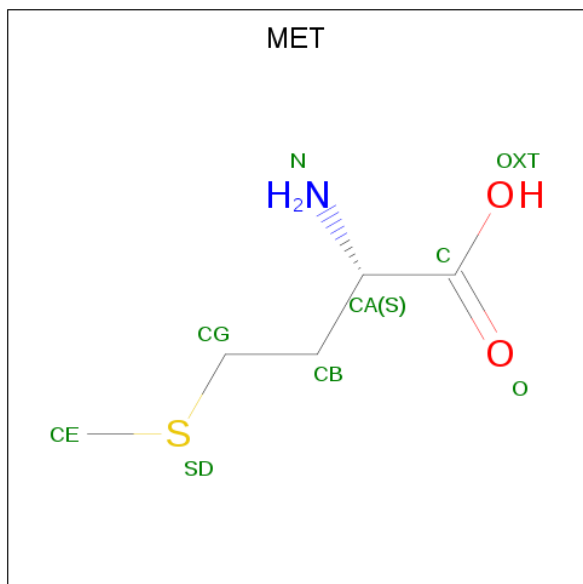
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0
			53	27	9	15	2	

Continued on next page...

Continued from previous page...

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

- Molecule 4 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
4	B	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

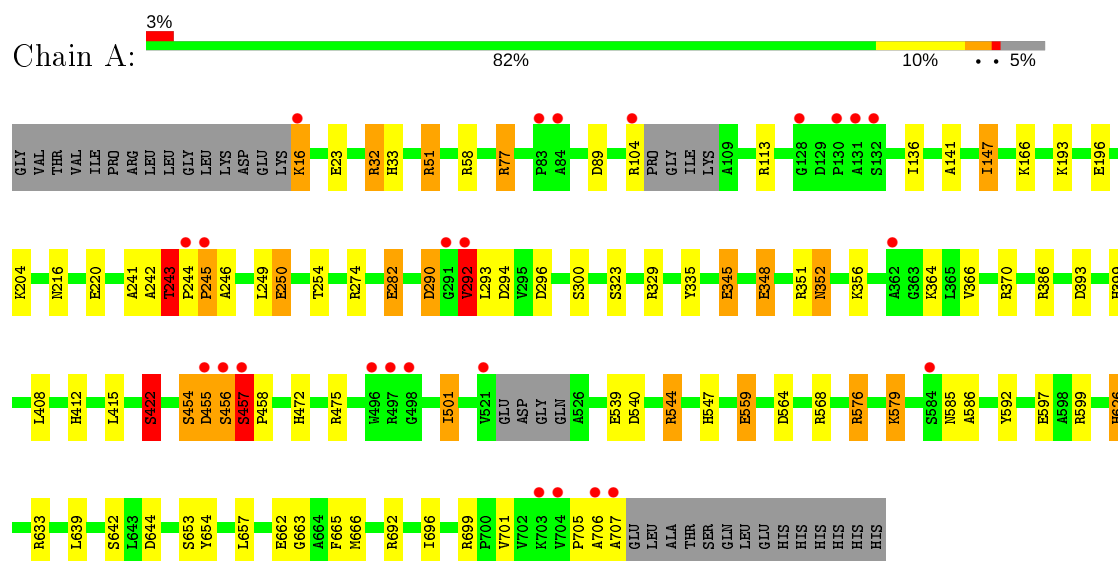
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1105	Total	O	0	0
			1105	1105		
6	B	1116	Total	O	0	0
			1116	1116		

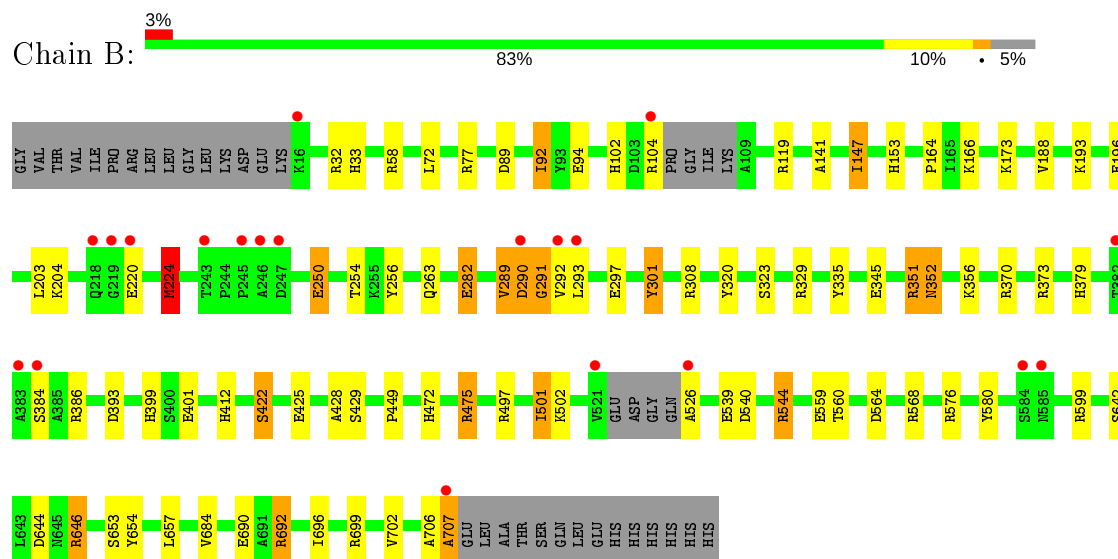
3 Residue-property plots [i](#)

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: Pro-enzyme of L-phenylalanine oxidase



- Molecule 1: Pro-enzyme of L-phenylalanine oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.27Å 112.84Å 136.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.27 – 1.25 36.26 – 1.25	Depositor EDS
% Data completeness (in resolution range)	97.0 (36.27-1.25) 97.1 (36.26-1.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 1.25Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.099 , 0.128 0.115 , 0.140	Depositor DCC
R_{free} test set	20873 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	9.3	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	12791	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, 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	1.32	45/5347 (0.8%)	1.41	54/7300 (0.7%)
1	B	1.23	40/5347 (0.7%)	1.39	52/7300 (0.7%)
All	All	1.28	85/10694 (0.8%)	1.40	106/14600 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	3
All	All	0	8

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	576	ARG	CD-NE	19.66	1.79	1.46
1	A	422	SER	CA-CB	18.44	1.80	1.52
1	B	544	ARG	CZ-NH2	-14.45	1.14	1.33
1	A	576	ARG	CZ-NH2	-13.89	1.15	1.33
1	B	544	ARG	CD-NE	13.32	1.69	1.46
1	B	297	GLU	CD-OE2	12.44	1.39	1.25
1	A	544	ARG	CD-NE	11.46	1.66	1.46
1	A	323	SER	CB-OG	-11.14	1.27	1.42
1	B	147	ILE	CA-CB	10.93	1.79	1.54
1	A	250	GLU	CG-CD	-10.71	1.35	1.51
1	B	301	TYR	CG-CD2	-10.58	1.25	1.39
1	A	544	ARG	CZ-NH2	-9.89	1.20	1.33
1	B	282	GLU	CD-OE2	9.45	1.36	1.25
1	A	544	ARG	NE-CZ	-9.39	1.20	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	GLU	CD-OE2	9.34	1.35	1.25
1	A	323	SER	CA-CB	9.00	1.66	1.52
1	A	243	THR	CA-C	8.96	1.76	1.52
1	B	323	SER	CA-CB	8.67	1.66	1.52
1	A	32	ARG	CG-CD	-8.37	1.31	1.51
1	A	559	GLU	CD-OE2	-7.99	1.16	1.25
1	B	301	TYR	CE2-CZ	-7.94	1.28	1.38
1	B	576	ARG	CZ-NH2	7.89	1.43	1.33
1	A	576	ARG	CZ-NH1	-7.67	1.23	1.33
1	B	282	GLU	CG-CD	7.66	1.63	1.51
1	A	23	GLU	CD-OE1	-7.46	1.17	1.25
1	B	323	SER	CB-OG	-7.41	1.32	1.42
1	A	282	GLU	CG-CD	7.39	1.63	1.51
1	A	422	SER	CB-OG	-7.37	1.32	1.42
1	B	560	THR	CA-CB	7.35	1.72	1.53
1	A	642	SER	CB-OG	7.31	1.51	1.42
1	B	544	ARG	CG-CD	7.26	1.70	1.51
1	B	642	SER	CB-OG	7.25	1.51	1.42
1	B	429	SER	CB-OG	-7.24	1.32	1.42
1	B	301	TYR	CD2-CE2	7.12	1.50	1.39
1	A	147	ILE	CB-CG2	7.08	1.74	1.52
1	A	242	ALA	CA-CB	7.00	1.67	1.52
1	A	568	ARG	NE-CZ	6.96	1.42	1.33
1	A	599	ARG	CZ-NH2	-6.94	1.24	1.33
1	A	345	GLU	CG-CD	6.91	1.62	1.51
1	A	579	LYS	CD-CE	6.89	1.68	1.51
1	A	559	GLU	CD-OE1	-6.85	1.18	1.25
1	B	422	SER	CA-CB	6.75	1.63	1.52
1	A	296	ASP	CB-CG	-6.71	1.37	1.51
1	A	586	ALA	CA-C	6.70	1.70	1.52
1	A	290	ASP	CB-CG	6.68	1.65	1.51
1	A	77	ARG	CZ-NH2	-6.60	1.24	1.33
1	A	597	GLU	CD-OE2	-6.54	1.18	1.25
1	A	352	ASN	CB-CG	-6.54	1.36	1.51
1	A	599	ARG	NE-CZ	6.42	1.41	1.33
1	B	250	GLU	CD-OE2	6.22	1.32	1.25
1	B	544	ARG	NE-CZ	-6.16	1.25	1.33
1	B	204	LYS	CE-NZ	-6.04	1.33	1.49
1	A	147	ILE	CA-CB	-6.04	1.41	1.54
1	B	263	GLN	CB-CG	-6.04	1.36	1.52
1	A	196	GLU	CG-CD	-6.00	1.43	1.51
1	B	386	ARG	CZ-NH1	6.00	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	599	ARG	CZ-NH2	-6.00	1.25	1.33
1	B	692	ARG	CZ-NH2	-5.98	1.25	1.33
1	B	580	TYR	CE1-CZ	-5.96	1.30	1.38
1	A	348	GLU	CB-CG	-5.93	1.40	1.52
1	A	568	ARG	CD-NE	-5.87	1.36	1.46
1	B	684	VAL	CB-CG2	-5.84	1.40	1.52
1	B	384	SER	CB-OG	-5.82	1.34	1.42
1	A	544	ARG	CG-CD	5.71	1.66	1.51
1	B	580	TYR	CZ-OH	-5.71	1.28	1.37
1	B	642	SER	CA-CB	5.69	1.61	1.52
1	A	576	ARG	NE-CZ	-5.60	1.25	1.33
1	A	345	GLU	CD-OE2	5.53	1.31	1.25
1	B	501	ILE	CG1-CD1	-5.52	1.12	1.50
1	B	301	TYR	CG-CD1	5.52	1.46	1.39
1	B	196	GLU	CG-CD	-5.51	1.43	1.51
1	A	457	SER	CA-CB	5.46	1.61	1.52
1	B	220	GLU	CG-CD	5.33	1.59	1.51
1	A	220	GLU	CB-CG	-5.27	1.42	1.52
1	B	32	ARG	CG-CD	-5.20	1.39	1.51
1	B	599	ARG	NE-CZ	5.16	1.39	1.33
1	B	568	ARG	CD-NE	-5.15	1.37	1.46
1	B	352	ASN	CB-CG	-5.09	1.39	1.51
1	A	243	THR	N-CA	5.07	1.56	1.46
1	B	699	ARG	CZ-NH1	5.05	1.39	1.33
1	B	188	VAL	CA-CB	5.05	1.65	1.54
1	A	241	ALA	CA-C	-5.03	1.39	1.52
1	B	559	GLU	CD-OE1	-5.02	1.20	1.25
1	A	292	VAL	N-CA	5.01	1.56	1.46
1	A	501	ILE	CG1-CD1	-5.01	1.16	1.50

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	386	ARG	NE-CZ-NH2	-41.03	99.78	120.30
1	A	576	ARG	NE-CZ-NH1	-33.91	103.34	120.30
1	A	576	ARG	CD-NE-CZ	-28.86	83.20	123.60
1	B	386	ARG	NE-CZ-NH1	28.05	134.33	120.30
1	B	544	ARG	NE-CZ-NH2	20.15	130.37	120.30
1	A	544	ARG	NE-CZ-NH2	18.41	129.51	120.30
1	A	77	ARG	NE-CZ-NH1	18.16	129.38	120.30
1	A	32	ARG	NE-CZ-NH1	18.15	129.37	120.30
1	B	699	ARG	NE-CZ-NH2	-17.33	111.63	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	576	ARG	NE-CZ-NH2	17.21	128.90	120.30
1	B	370	ARG	NE-CZ-NH2	-16.88	111.86	120.30
1	B	699	ARG	NE-CZ-NH1	16.80	128.70	120.30
1	B	568	ARG	NE-CZ-NH1	16.69	128.65	120.30
1	A	77	ARG	NE-CZ-NH2	-15.04	112.78	120.30
1	A	599	ARG	NE-CZ-NH2	-14.09	113.26	120.30
1	B	544	ARG	NE-CZ-NH1	-14.02	113.29	120.30
1	A	351	ARG	NE-CZ-NH1	13.74	127.17	120.30
1	A	599	ARG	NE-CZ-NH1	13.66	127.13	120.30
1	B	599	ARG	NE-CZ-NH1	13.64	127.12	120.30
1	A	544	ARG	NE-CZ-NH1	-13.20	113.70	120.30
1	A	692	ARG	NE-CZ-NH2	-12.98	113.81	120.30
1	B	646	ARG	NE-CZ-NH1	12.66	126.63	120.30
1	A	455	ASP	CB-CG-OD1	-11.82	107.66	118.30
1	B	351	ARG	NE-CZ-NH1	11.67	126.14	120.30
1	A	576	ARG	NH1-CZ-NH2	11.62	132.18	119.40
1	B	370	ARG	NE-CZ-NH1	10.85	125.73	120.30
1	B	386	ARG	CD-NE-CZ	10.28	137.99	123.60
1	A	370	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	A	568	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	B	599	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	B	568	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	A	592	TYR	CB-CG-CD2	9.03	126.42	121.00
1	A	559	GLU	OE1-CD-OE2	-9.01	112.49	123.30
1	B	576	ARG	NE-CZ-NH1	-8.84	115.88	120.30
1	A	457	SER	C-N-CD	8.82	146.92	128.40
1	B	692	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	A	290	ASP	CB-CG-OD1	8.59	126.03	118.30
1	B	692	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	A	58	ARG	NE-CZ-NH2	8.21	124.41	120.30
1	A	701	VAL	CG1-CB-CG2	8.13	123.92	110.90
1	B	646	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	A	113	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	564	ASP	CB-CG-OD1	7.77	125.29	118.30
1	A	293	LEU	CB-CG-CD1	7.70	124.09	111.00
1	B	475	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	A	501	ILE	CB-CG1-CD1	7.46	134.77	113.90
1	A	32	ARG	NH1-CZ-NH2	-7.45	111.20	119.40
1	A	633	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	B	58	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	B	564	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	B	256	TYR	CZ-CE2-CD2	-7.14	113.37	119.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	633	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	A	626	HIS	CG-ND1-CE1	-6.73	96.95	105.70
1	A	294	ASP	CB-CG-OD1	6.62	124.26	118.30
1	A	699	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	348	GLU	OE1-CD-OE2	-6.55	115.44	123.30
1	B	707	ALA	CB-CA-C	-6.51	100.34	110.10
1	A	576	ARG	NE-CZ-NH2	6.43	123.52	120.30
1	A	243	THR	CA-CB-CG2	6.31	121.23	112.40
1	B	92	ILE	CA-CB-CG1	6.28	122.93	111.00
1	B	329	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	A	386	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	B	320	TYR	CB-CG-CD1	6.21	124.72	121.00
1	B	289	VAL	C-N-CA	-6.17	106.28	121.70
1	B	256	TYR	CE1-CZ-CE2	6.14	129.62	119.80
1	A	699	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	119	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	455	ASP	O-C-N	-6.05	113.03	122.70
1	A	113	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	568	ARG	NH1-CZ-NH2	-6.00	112.81	119.40
1	A	544	ARG	CG-CD-NE	5.99	124.39	111.80
1	A	345	GLU	CA-CB-CG	5.95	126.48	113.40
1	B	501	ILE	CB-CG1-CD1	5.94	130.54	113.90
1	A	692	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	425	GLU	OE1-CD-OE2	-5.77	116.37	123.30
1	A	364	LYS	CD-CE-NZ	-5.71	98.56	111.70
1	A	422	SER	CA-CB-OG	-5.66	95.93	111.20
1	B	119	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	B	373	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	497	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	351	ARG	CD-NE-CZ	5.59	131.42	123.60
1	A	456	SER	N-CA-CB	-5.52	102.22	110.50
1	B	203	LEU	CB-CG-CD1	5.52	120.39	111.00
1	A	351	ARG	NH1-CZ-NH2	-5.52	113.33	119.40
1	B	224	MET	CG-SD-CE	-5.48	91.43	100.20
1	B	290	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	B	644	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	A	89	ASP	CB-CG-OD1	5.43	123.19	118.30
1	B	308	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	568	ARG	CG-CD-NE	-5.41	100.45	111.80
1	A	329	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	386	ARG	NH1-CZ-NH2	5.40	125.34	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	329	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	457	SER	CB-CA-C	-5.33	99.97	110.10
1	B	544	ARG	CG-CD-NE	5.33	122.99	111.80
1	B	173	LYS	CD-CE-NZ	5.32	123.92	111.70
1	A	455	ASP	OD1-CG-OD2	5.21	133.20	123.30
1	A	58	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	B	256	TYR	CD1-CE1-CZ	-5.15	115.16	119.80
1	B	475	ARG	CD-NE-CZ	5.11	130.76	123.60
1	B	89	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	166	LYS	CD-CE-NZ	5.08	123.39	111.70
1	B	690	GLU	OE1-CD-OE2	-5.06	117.23	123.30
1	B	568	ARG	CD-NE-CZ	5.05	130.67	123.60
1	A	51	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	THR	Mainchain
1	A	245	PRO	Peptide
1	A	335	TYR	Sidechain
1	A	454	SER	Peptide
1	A	654	TYR	Sidechain
1	B	335	TYR	Sidechain
1	B	654	TYR	Sidechain
1	B	706	ALA	Peptide

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	5212	0	5100	105	0
1	B	5212	0	5102	88	1
2	A	10	0	0	0	0
3	A	53	0	31	2	0
3	B	53	0	31	2	0
4	A	9	0	8	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	9	0	8	1	0
5	A	6	0	8	0	0
5	B	6	0	7	0	0
6	A	1105	0	0	78	11
6	B	1116	0	0	40	10
All	All	12791	0	10295	191	11

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 9.

All (191) 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:147:ILE:CG2	1:A:147:ILE:CB	1.74	1.63
1:A:422:SER:CB	1:A:422:SER:CA	1.80	1.58
1:B:147:ILE:CB	1:B:147:ILE:CA	1.80	1.55
1:A:243:THR:CA	1:A:243:THR:C	1.76	1.54
1:B:544:ARG:NE	1:B:544:ARG:CD	1.69	1.52
1:B:290:ASP:OD2	1:B:292:VAL:HG12	1.24	1.27
1:A:250:GLU:HG2	6:A:7114:HOH:O	1.24	1.27
1:B:707:ALA:HA	6:B:6657:HOH:O	1.08	1.24
1:A:707:ALA:HA	6:A:7149:HOH:O	1.38	1.23
1:B:352:ASN:HB3	6:B:7113:HOH:O	1.07	1.22
1:A:626:HIS:CD2	6:A:7207:HOH:O	1.95	1.18
1:A:352:ASN:HB3	6:A:7112:HOH:O	1.03	1.17
1:B:356:LYS:HE2	6:B:7147:HOH:O	1.45	1.16
1:B:707:ALA:HB2	6:B:6448:HOH:O	1.47	1.15
1:B:475:ARG:HD2	6:B:7144:HOH:O	1.44	1.14
1:A:662:GLU:O	6:A:7200:HOH:O	1.62	1.12
1:A:16:LYS:HA	6:A:7093:HOH:O	1.48	1.11
1:B:290:ASP:OD2	1:B:292:VAL:CG1	1.99	1.10
1:B:164:PRO:HG2	6:B:6333:HOH:O	1.50	1.08
1:B:290:ASP:OD1	1:B:293:LEU:N	1.89	1.05
1:B:290:ASP:CG	1:B:292:VAL:HG12	1.78	1.04
1:A:576:ARG:NE	6:A:7117:HOH:O	1.89	1.04
1:B:282:GLU:HG3	6:B:6146:HOH:O	1.57	1.03
1:B:293:LEU:O	6:B:7089:HOH:O	1.74	1.03
1:B:702:VAL:HG22	6:B:7203:HOH:O	0.85	1.02
1:A:707:ALA:CB	6:A:7119:HOH:O	2.07	1.01
1:A:665:PHE:N	6:A:7200:HOH:O	1.95	0.97
1:A:707:ALA:HA	6:A:7119:HOH:O	1.65	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ARG:HA	6:B:6433:HOH:O	1.65	0.96
1:A:77:ARG:HD2	6:A:6229:HOH:O	1.65	0.95
1:A:282:GLU:HG3	6:A:5838:HOH:O	1.67	0.93
1:B:379:HIS:HE1	1:B:646:ARG:H	1.15	0.93
6:A:7169:HOH:O	1:B:301:TYR:CE1	2.19	0.93
1:A:475:ARG:HD2	6:A:7140:HOH:O	1.70	0.90
1:B:301:TYR:HE2	6:B:6018:HOH:O	1.54	0.89
1:A:348:GLU:CD	6:A:7059:HOH:O	2.09	0.89
1:B:290:ASP:OD1	1:B:292:VAL:N	2.05	0.89
1:A:707:ALA:HB1	6:A:5399:HOH:O	1.74	0.88
1:B:544:ARG:CZ	1:B:544:ARG:CD	2.52	0.88
1:A:104:ARG:O	6:A:6633:HOH:O	1.91	0.87
1:A:250:GLU:OE1	6:A:7163:HOH:O	1.91	0.86
1:A:250:GLU:OE1	6:A:6189:HOH:O	1.93	0.85
1:B:292:VAL:HG11	6:B:6232:HOH:O	1.76	0.84
1:B:193:LYS:HD2	6:B:6014:HOH:O	1.76	0.84
1:B:301:TYR:CE2	6:B:6018:HOH:O	2.31	0.82
1:B:290:ASP:OD1	1:B:292:VAL:CA	2.28	0.81
1:A:422:SER:HB3	6:A:5663:HOH:O	1.78	0.81
1:A:706:ALA:O	1:A:707:ALA:HB2	1.81	0.80
1:B:147:ILE:CA	1:B:147:ILE:CG1	2.62	0.77
1:A:696:ILE:HD11	6:A:6409:HOH:O	1.86	0.76
1:A:147:ILE:HB	1:A:147:ILE:CG2	2.11	0.75
1:B:147:ILE:CA	1:B:147:ILE:HD13	2.16	0.75
1:A:250:GLU:CG	6:A:7114:HOH:O	1.99	0.75
1:A:147:ILE:CG1	1:A:147:ILE:CG2	2.63	0.75
1:A:472:HIS:HE1	1:A:539:GLU:OE2	1.69	0.74
1:B:290:ASP:OD1	1:B:292:VAL:C	2.26	0.74
6:A:6438:HOH:O	1:B:301:TYR:CE1	2.39	0.74
1:A:422:SER:OG	1:A:422:SER:CA	2.34	0.74
1:A:254:THR:HG22	6:A:6059:HOH:O	1.87	0.73
1:A:576:ARG:CZ	6:A:7117:HOH:O	2.27	0.73
1:A:540:ASP:OD2	1:B:472:HIS:HD2	1.71	0.73
1:B:147:ILE:HD13	1:B:147:ILE:HA	1.70	0.73
1:B:472:HIS:HE1	1:B:539:GLU:OE2	1.71	0.73
1:B:422:SER:HB3	6:B:7168:HOH:O	1.89	0.73
1:B:290:ASP:CG	1:B:292:VAL:H	1.91	0.72
1:B:352:ASN:OD1	6:B:7125:HOH:O	2.06	0.72
1:A:472:HIS:HD2	1:B:540:ASP:OD2	1.72	0.72
1:B:290:ASP:CG	1:B:292:VAL:CG1	2.52	0.71
1:A:707:ALA:HB1	6:A:7119:HOH:O	1.80	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:HIS:NE2	6:A:7207:HOH:O	2.08	0.70
1:A:104:ARG:CG	6:A:6780:HOH:O	2.39	0.69
1:A:352:ASN:OD1	6:A:6673:HOH:O	2.09	0.69
1:A:104:ARG:CB	6:A:6780:HOH:O	2.39	0.69
1:A:104:ARG:HG2	6:A:6780:HOH:O	1.92	0.69
1:A:352:ASN:ND2	6:A:7102:HOH:O	2.26	0.68
1:A:626:HIS:HD2	6:A:5843:HOH:O	1.76	0.68
1:A:663:GLY:C	6:A:7200:HOH:O	2.31	0.68
1:B:544:ARG:HD2	6:B:5810:HOH:O	1.94	0.68
1:B:544:ARG:NH1	1:B:544:ARG:CD	2.57	0.68
1:A:626:HIS:CD2	6:A:5843:HOH:O	2.46	0.67
1:B:475:ARG:CD	6:B:7144:HOH:O	2.17	0.67
1:A:544:ARG:NH1	6:A:6511:HOH:O	2.27	0.67
1:B:147:ILE:CA	1:B:147:ILE:CD1	2.72	0.67
1:B:526:ALA:N	6:B:7009:HOH:O	2.28	0.66
1:A:706:ALA:O	1:A:707:ALA:CB	2.43	0.66
6:A:7169:HOH:O	1:B:301:TYR:HE1	1.68	0.66
1:B:250:GLU:OE2	1:B:254:THR:HG21	1.96	0.66
1:B:292:VAL:CG1	6:B:6232:HOH:O	2.39	0.66
1:B:544:ARG:CD	1:B:544:ARG:HH11	2.08	0.65
1:A:707:ALA:CA	6:A:7119:HOH:O	2.17	0.65
1:B:393:ASP:OD2	1:B:399:HIS:HE1	1.79	0.65
1:B:544:ARG:NH1	6:B:7111:HOH:O	2.29	0.65
1:A:666:MET:N	6:A:7200:HOH:O	2.10	0.64
1:A:254:THR:HG21	6:A:6189:HOH:O	1.95	0.64
1:B:379:HIS:CE1	1:B:646:ARG:H	2.07	0.64
1:A:455:ASP:HB3	6:A:6271:HOH:O	1.97	0.64
1:A:644:ASP:OD1	6:A:6038:HOH:O	2.15	0.64
1:A:705:PRO:HG3	6:A:5555:HOH:O	1.96	0.64
1:A:639:LEU:O	1:A:707:ALA:HB3	1.98	0.63
1:B:412:HIS:HD2	1:B:653:SER:OG	1.81	0.63
1:B:254:THR:HG22	6:B:6631:HOH:O	1.99	0.63
1:A:243:THR:HG23	6:A:5998:HOH:O	1.98	0.63
1:A:412:HIS:HD2	1:A:653:SER:OG	1.83	0.62
6:A:7090:HOH:O	1:B:293:LEU:HD23	1.98	0.62
1:A:544:ARG:HD2	6:A:5635:HOH:O	1.99	0.62
1:A:626:HIS:HE1	6:A:5463:HOH:O	1.83	0.61
1:A:422:SER:CB	1:A:422:SER:N	2.58	0.61
1:A:585:ASN:ND2	1:B:428:ALA:H	1.99	0.61
1:B:289:VAL:HB	1:B:293:LEU:HD12	1.83	0.61
1:A:579:LYS:NZ	6:A:7221:HOH:O	2.20	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ARG:CD	6:A:7140:HOH:O	2.39	0.60
1:A:16:LYS:N	6:A:6193:HOH:O	2.34	0.60
1:A:454:SER:HG	1:A:456:SER:H	1.49	0.59
1:B:702:VAL:CG2	6:B:7203:HOH:O	1.71	0.59
1:A:290:ASP:HB3	1:A:292:VAL:CG1	2.33	0.59
1:B:102:HIS:HD2	6:B:5559:HOH:O	1.84	0.58
1:A:193:LYS:HD2	6:A:5755:HOH:O	2.02	0.58
1:B:696:ILE:HD11	6:B:6107:HOH:O	2.02	0.58
1:A:104:ARG:C	6:A:6780:HOH:O	2.42	0.58
1:A:457:SER:O	1:A:458:PRO:C	2.41	0.57
1:A:193:LYS:CE	6:A:6672:HOH:O	2.53	0.57
1:A:639:LEU:O	1:A:707:ALA:CB	2.54	0.56
1:A:662:GLU:C	6:A:7200:HOH:O	2.26	0.56
1:B:290:ASP:C	1:B:292:VAL:N	2.58	0.56
1:A:51:ARG:NH1	6:A:7148:HOH:O	2.31	0.56
1:A:626:HIS:CE1	6:A:5883:HOH:O	2.59	0.54
1:B:153:HIS:HE1	6:B:6097:HOH:O	1.89	0.54
1:A:559:GLU:OE2	6:A:7141:HOH:O	2.18	0.53
1:B:290:ASP:OD1	1:B:292:VAL:CG1	2.56	0.53
1:A:246:ALA:HA	6:A:6402:HOH:O	2.08	0.53
1:A:422:SER:CB	1:A:422:SER:C	2.71	0.53
1:B:282:GLU:CG	6:B:6146:HOH:O	2.33	0.52
1:A:104:ARG:HB3	6:A:6780:HOH:O	2.07	0.52
1:B:292:VAL:CB	6:B:6232:HOH:O	2.57	0.52
1:A:399:HIS:HD2	6:A:6204:HOH:O	1.93	0.51
1:A:422:SER:HB2	6:A:7146:HOH:O	2.10	0.51
1:B:224:MET:HE3	6:B:6453:HOH:O	2.10	0.51
1:B:356:LYS:HE2	6:B:7082:HOH:O	2.10	0.50
1:A:147:ILE:CA	1:A:147:ILE:CG2	2.73	0.50
1:A:393:ASP:OD2	1:A:399:HIS:HE1	1.93	0.50
1:A:626:HIS:CE1	6:A:5463:HOH:O	2.61	0.50
1:B:707:ALA:N	6:B:6657:HOH:O	2.31	0.50
1:B:147:ILE:CB	1:B:147:ILE:N	2.68	0.50
1:A:243:THR:CB	1:A:243:THR:C	2.74	0.50
1:A:243:THR:C	1:A:243:THR:HA	2.14	0.49
1:B:193:LYS:HE3	6:B:5602:HOH:O	2.11	0.49
1:B:147:ILE:CA	1:B:147:ILE:CG2	2.83	0.49
1:B:141:ALA:HA	3:B:801:FAD:C4X	2.43	0.49
1:B:401:GLU:OE2	6:B:6212:HOH:O	2.20	0.49
1:A:216:ASN:OD1	6:A:6397:HOH:O	2.19	0.49
1:B:94:GLU:O	1:B:102:HIS:HE1	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:HIS:CE1	1:A:657:LEU:HD11	2.48	0.48
1:B:526:ALA:CA	6:B:7009:HOH:O	2.59	0.48
1:B:33:HIS:CE1	1:B:657:LEU:HD11	2.48	0.48
1:A:51:ARG:NH2	6:A:7148:HOH:O	2.32	0.48
1:B:193:LYS:CE	6:B:5602:HOH:O	2.62	0.47
1:A:454:SER:OG	1:A:456:SER:N	2.32	0.47
1:A:244:PRO:HG2	1:A:249:LEU:HD11	1.97	0.46
1:A:16:LYS:CA	6:A:7093:HOH:O	2.31	0.46
3:B:801:FAD:N5	4:B:1905:MET:HA	2.30	0.46
1:B:147:ILE:CB	1:B:147:ILE:C	2.72	0.46
1:B:290:ASP:C	1:B:292:VAL:H	2.19	0.46
1:A:193:LYS:N	1:A:193:LYS:HD3	2.30	0.45
6:A:7169:HOH:O	1:B:301:TYR:CD1	2.59	0.45
1:B:692:ARG:NH1	6:B:6998:HOH:O	2.48	0.45
1:A:457:SER:OG	1:B:290:ASP:OD2	2.18	0.45
1:A:32:ARG:NE	6:A:5798:HOH:O	2.50	0.44
1:B:72:LEU:HD22	1:B:92:ILE:HD11	2.00	0.44
1:A:141:ALA:HA	3:A:801:FAD:C4X	2.47	0.44
1:A:356:LYS:HD3	6:A:6126:HOH:O	2.18	0.44
1:A:300:SER:HB3	6:A:7202:HOH:O	2.17	0.44
1:B:351:ARG:NH1	6:B:6965:HOH:O	2.39	0.44
1:A:243:THR:CG2	6:A:5373:HOH:O	2.65	0.43
1:A:585:ASN:ND2	6:A:5709:HOH:O	2.51	0.43
1:B:502:LYS:NZ	6:B:7116:HOH:O	2.05	0.43
3:A:801:FAD:N5	4:A:905:MET:HA	2.34	0.43
1:A:245:PRO:HB3	6:A:5905:HOH:O	2.19	0.43
1:A:547:HIS:HE1	6:A:6618:HOH:O	2.01	0.43
1:B:164:PRO:CG	6:B:6333:HOH:O	2.30	0.42
1:A:408:LEU:HD13	1:A:415:LEU:HD11	2.01	0.42
1:A:274:ARG:NH2	6:A:7202:HOH:O	2.29	0.42
1:B:379:HIS:HD2	1:B:449:PRO:O	2.03	0.42
1:A:193:LYS:CD	6:A:6672:HOH:O	2.68	0.42
1:B:526:ALA:HA	6:B:7009:HOH:O	2.20	0.41
6:A:7090:HOH:O	1:B:293:LEU:CD2	2.64	0.41
1:A:244:PRO:HG2	1:A:249:LEU:CD1	2.50	0.41
1:A:104:ARG:NE	6:A:6780:HOH:O	2.53	0.41
1:A:366:VAL:HG12	6:A:6686:HOH:O	2.21	0.41
1:B:166:LYS:HE3	1:B:166:LYS:HB2	1.91	0.40
1:A:136:ILE:HD12	1:A:345:GLU:HG2	2.04	0.40
1:B:290:ASP:O	1:B:291:GLY:C	2.60	0.40

All (11) 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)
6:A:7178:HOH:O	6:B:5799:HOH:O[4_556]	1.59	0.61
6:A:7170:HOH:O	6:B:6908:HOH:O[3_756]	1.62	0.58
6:A:7004:HOH:O	6:B:5927:HOH:O[2_664]	1.93	0.27
6:A:5623:HOH:O	6:B:6908:HOH:O[3_756]	1.95	0.25
6:A:7036:HOH:O	6:B:7205:HOH:O[4_556]	1.99	0.21
6:A:6939:HOH:O	6:B:5921:HOH:O[3_756]	2.03	0.17
6:A:7221:HOH:O	6:B:6868:HOH:O[2_664]	2.05	0.15
6:A:7036:HOH:O	6:B:5956:HOH:O[4_556]	2.08	0.12
6:A:7178:HOH:O	6:B:6636:HOH:O[4_556]	2.11	0.09
6:A:7010:HOH:O	6:B:6861:HOH:O[3_756]	2.12	0.08
1:B:193:LYS:NZ	6:A:7177:HOH:O[2_665]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	678/721 (94%)	658 (97%)	20 (3%)	0	100	100
1	B	678/721 (94%)	662 (98%)	15 (2%)	1 (0%)	51	19
All	All	1356/1442 (94%)	1320 (97%)	35 (3%)	1 (0%)	51	19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	291	GLY

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	534/566 (94%)	527 (99%)	7 (1%)	69	32
1	B	534/566 (94%)	531 (99%)	3 (1%)	86	62
All	All	1068/1132 (94%)	1058 (99%)	10 (1%)	78	47

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	204	LYS
1	A	243	THR
1	A	292	VAL
1	A	422	SER
1	A	457	SER
1	A	501	ILE
1	B	224	MET
1	B	345	GLU
1	B	501	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	ASN
1	A	399	HIS
1	A	412	HIS
1	A	472	HIS
1	A	585	ASN
1	A	626	HIS
1	B	102	HIS
1	B	153	HIS
1	B	263	GLN
1	B	337	ASN
1	B	379	HIS
1	B	396	ASN
1	B	399	HIS
1	B	412	HIS
1	B	472	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
5	GOL	A	902	-	5,5,5	0.72	0	5,5,5	0.62	0
3	FAD	A	801	-	51,58,58	1.46	7 (13%)	60,89,89	2.00	10 (16%)
3	FAD	B	801	-	51,58,58	1.60	7 (13%)	60,89,89	1.73	10 (16%)
5	GOL	B	1902	-	5,5,5	1.02	0	5,5,5	0.70	0
2	SO4	A	3001	-	4,4,4	1.54	1 (25%)	6,6,6	4.45	5 (83%)
2	SO4	A	3002	-	4,4,4	0.95	0	6,6,6	3.28	2 (33%)

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
3	FAD	A	801	-	-	5/30/50/50	0/6/6/6
5	GOL	A	902	-	-	0/4/4/4	-
3	FAD	B	801	-	-	3/30/50/50	0/6/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	1902	-	-	0/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	FAD	C4X-N5	5.28	1.40	1.33
3	A	801	FAD	C4X-N5	4.86	1.40	1.33
3	B	801	FAD	O4B-C1B	4.51	1.47	1.41
3	A	801	FAD	C4-N3	3.91	1.39	1.33
3	B	801	FAD	C4-C4X	-3.61	1.35	1.41
3	B	801	FAD	C4-N3	3.32	1.38	1.33
3	A	801	FAD	C4-C4X	-3.31	1.35	1.41
3	B	801	FAD	C2-N1	-2.86	1.32	1.38
2	A	3001	SO4	O4-S	-2.67	1.26	1.47
3	A	801	FAD	C5'-C4'	2.62	1.55	1.51
3	A	801	FAD	C6-C5X	-2.40	1.38	1.41
3	B	801	FAD	C5X-N5	2.31	1.39	1.35
3	A	801	FAD	C5X-N5	2.27	1.39	1.35
3	B	801	FAD	C4X-C10	2.18	1.41	1.38
3	A	801	FAD	C4X-C10	-2.01	1.36	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	FAD	C4-N3-C2	10.57	124.07	115.14
2	A	3001	SO4	O3-S-O1	-8.10	67.01	109.31
3	B	801	FAD	C4-N3-C2	7.51	121.48	115.14
2	A	3002	SO4	O3-S-O2	-6.22	76.84	109.31
3	A	801	FAD	C4X-C4-N3	-5.49	115.92	123.43
2	A	3002	SO4	O2-S-O1	4.83	145.14	109.43
2	A	3001	SO4	O4-S-O1	-4.29	86.93	109.31
2	A	3001	SO4	O4-S-O3	4.19	126.95	109.06
3	A	801	FAD	C1'-N10-C9A	3.96	121.41	118.29
3	B	801	FAD	C4X-C4-N3	-3.53	118.61	123.43
3	B	801	FAD	C4-C4X-N5	3.52	122.63	118.60
2	A	3001	SO4	O4-S-O2	3.45	127.33	109.31
3	B	801	FAD	C5'-C4'-C3'	-3.16	106.10	112.20
3	B	801	FAD	C1'-N10-C9A	2.99	120.65	118.29
3	B	801	FAD	C10-C4X-N5	-2.93	119.23	121.26
3	B	801	FAD	O4B-C1B-C2B	-2.82	102.80	106.93
3	B	801	FAD	C4-C4X-C10	-2.77	118.12	119.95
3	A	801	FAD	C4X-N5-C5X	2.57	119.34	116.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	FAD	C3B-C2B-C1B	2.53	104.78	100.98
3	B	801	FAD	C5A-C6A-N6A	2.51	124.16	120.35
3	A	801	FAD	C9A-C5X-N5	-2.43	118.56	122.36
3	A	801	FAD	C5'-C4'-C3'	-2.37	107.63	112.20
3	A	801	FAD	C5X-C9A-N10	2.34	119.41	117.72
3	B	801	FAD	C4X-N5-C5X	2.29	119.06	116.77
3	A	801	FAD	C9-C9A-C5X	-2.28	115.99	119.88
2	A	3001	SO4	O2-S-O1	2.18	125.50	109.43
3	A	801	FAD	O2P-P-O1P	2.06	122.42	112.24

There are no chirality outliers.

All (8) torsion outliers are listed below:

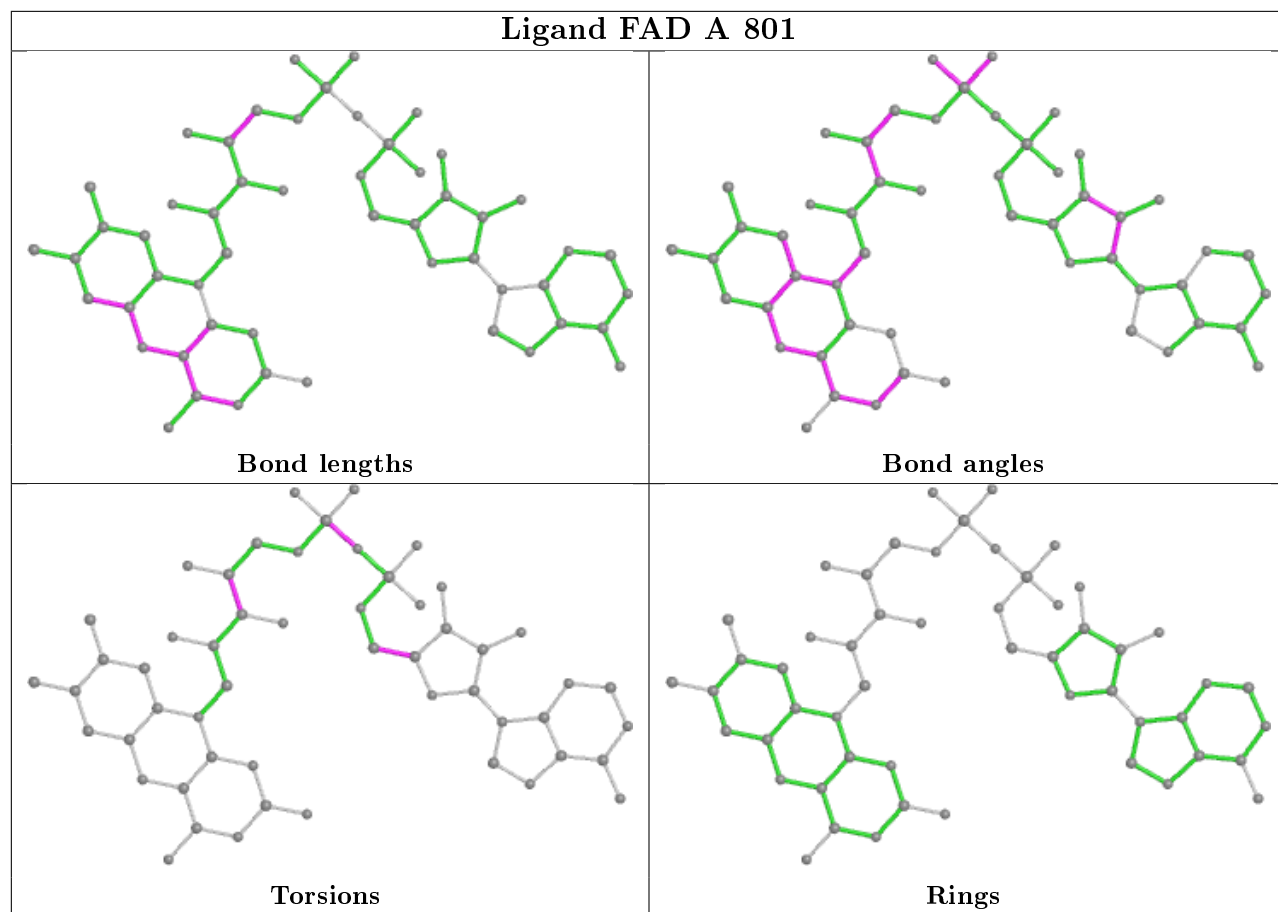
Mol	Chain	Res	Type	Atoms
3	A	801	FAD	PA-O3P-P-O5'
3	B	801	FAD	PA-O3P-P-O5'
3	A	801	FAD	C2'-C3'-C4'-C5'
3	A	801	FAD	C2'-C3'-C4'-O4'
3	B	801	FAD	C2'-C3'-C4'-O4'
3	B	801	FAD	O4B-C4B-C5B-O5B
3	A	801	FAD	O4B-C4B-C5B-O5B
3	A	801	FAD	O3'-C3'-C4'-C5'

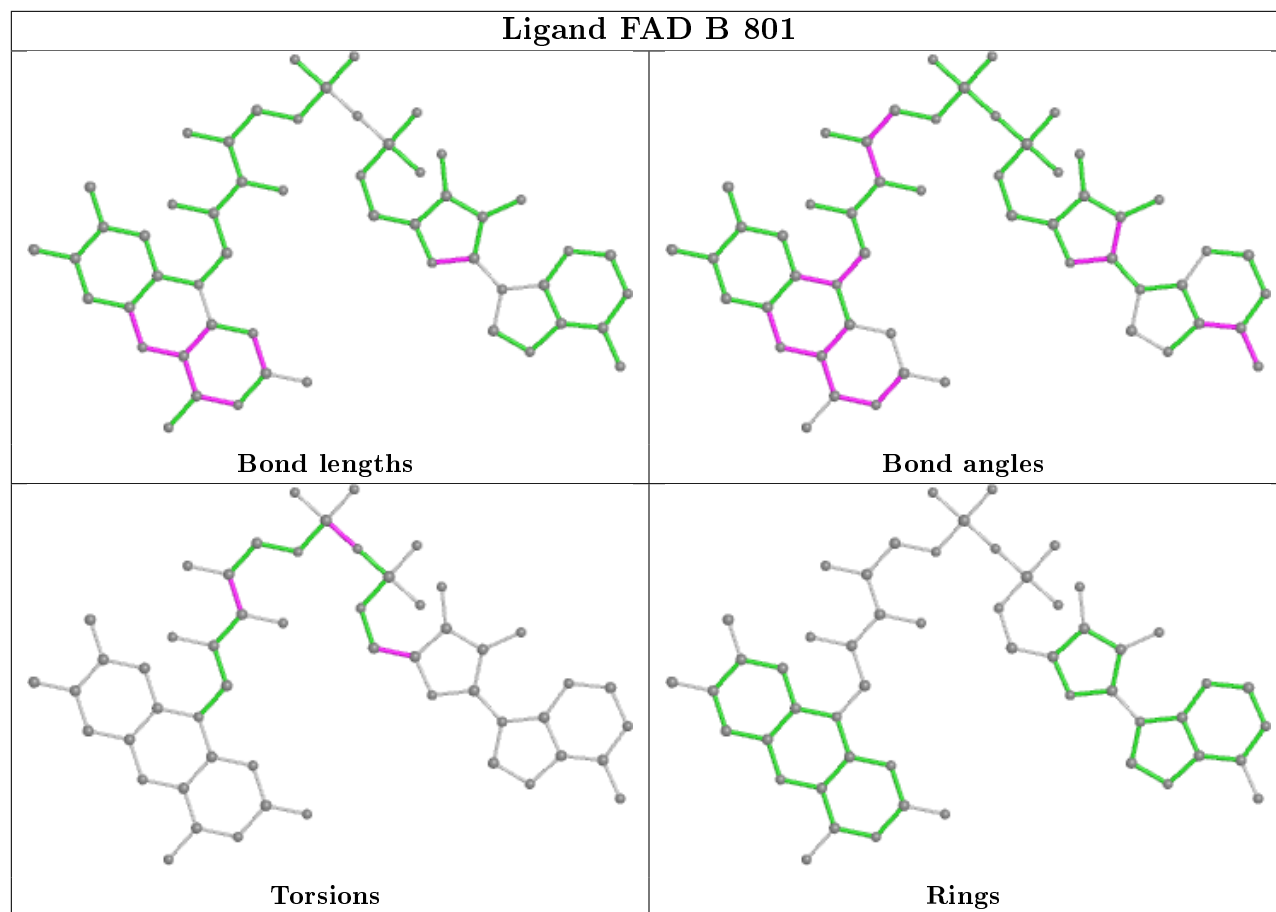
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	FAD	2	0
3	B	801	FAD	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	684/721 (94%)	-0.36	25 (3%) 41 34	6, 11, 25, 43	0
1	B	684/721 (94%)	-0.40	20 (2%) 51 44	6, 11, 24, 42	0
All	All	1368/1442 (94%)	-0.38	45 (3%) 46 38	6, 11, 25, 43	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	707	ALA	9.1
1	B	292	VAL	8.3
1	A	104	ARG	7.2
1	A	362	ALA	6.6
1	B	293	LEU	6.3
1	B	707	ALA	5.7
1	B	521	VAL	5.7
1	A	521	VAL	5.6
1	A	131	ALA	4.5
1	B	585	ASN	4.5
1	A	292	VAL	4.4
1	B	218	GLN	3.7
1	A	245	PRO	3.7
1	A	132	SER	3.7
1	A	456	SER	3.7
1	B	246	ALA	3.6
1	A	16	LYS	3.6
1	A	706	ALA	3.3
1	B	104	ARG	3.3
1	A	498	GLY	3.3
1	B	526	ALA	3.3
1	B	290	ASP	3.0
1	A	291	GLY	2.9
1	A	128	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	584	SER	2.9
1	A	130	PRO	2.8
1	A	496	TRP	2.7
1	A	244	PRO	2.7
1	B	382	THR	2.7
1	A	84	ALA	2.5
1	B	16	LYS	2.5
1	B	383	ALA	2.5
1	B	243	THR	2.4
1	B	220	GLU	2.4
1	A	704	VAL	2.4
1	A	457	SER	2.3
1	B	384	SER	2.3
1	A	83	PRO	2.3
1	A	455	ASP	2.3
1	B	219	GLY	2.3
1	A	584	SER	2.2
1	B	247	ASP	2.2
1	B	245	PRO	2.1
1	A	497	ARG	2.1
1	A	703	LYS	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, 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.

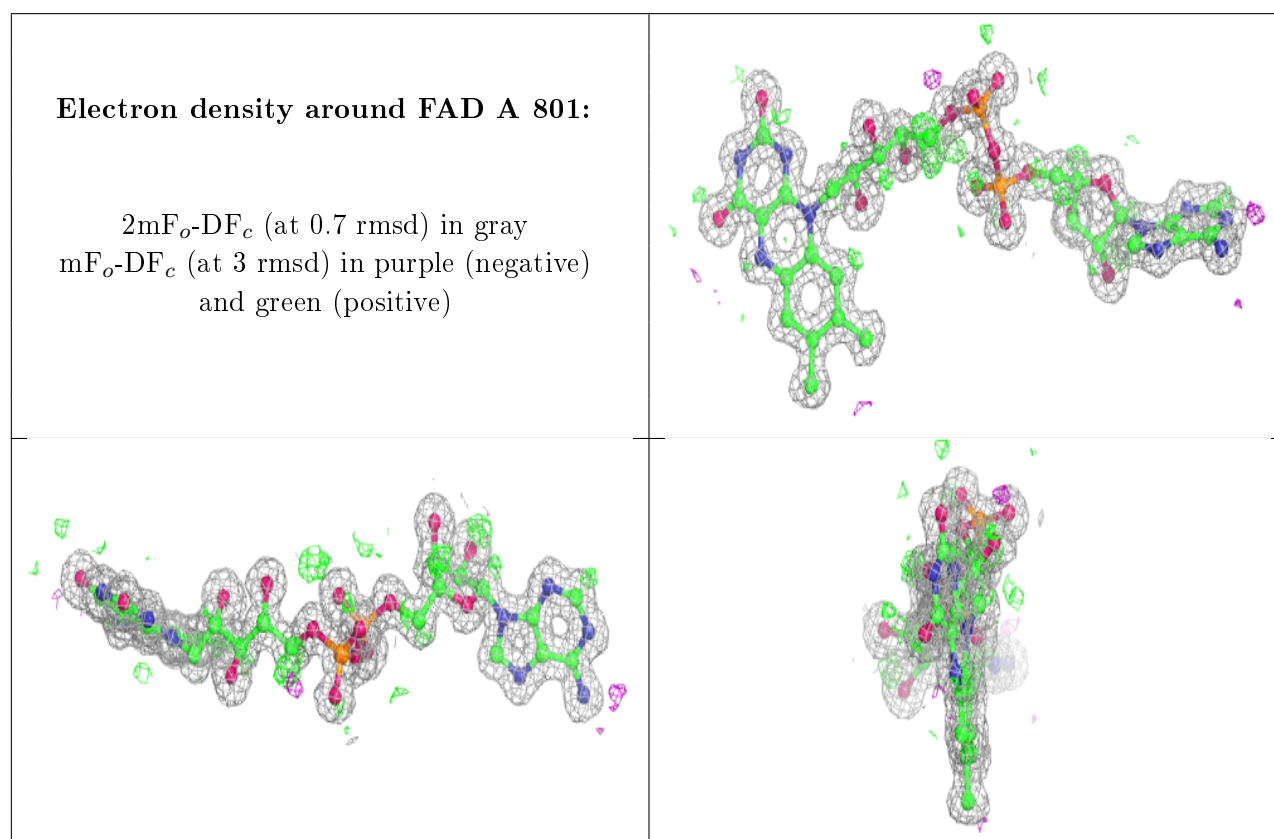
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	A	3001	5/5	0.96	0.15	16,17,28,32	0
5	GOL	B	1902	6/6	0.98	0.04	10,11,13,16	0

Continued on next page...

Continued from previous page...

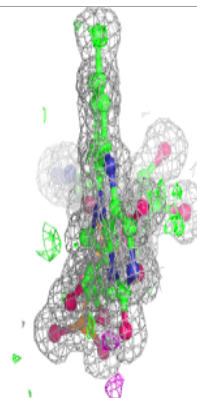
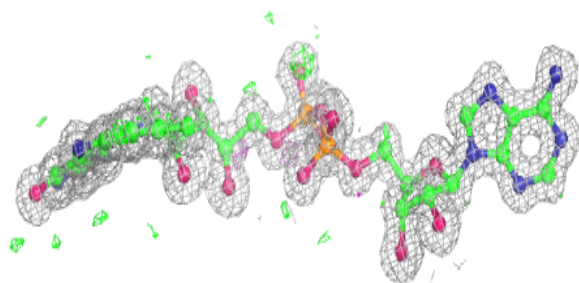
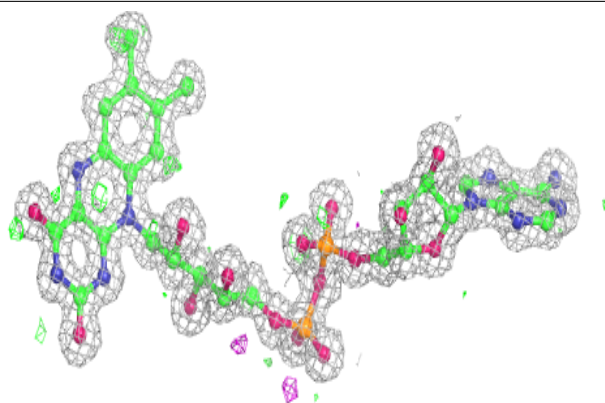
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MET	A	905	9/9	0.98	0.05	8,9,14,15	0
4	MET	B	1905	9/9	0.98	0.06	9,10,14,14	0
5	GOL	A	902	6/6	0.98	0.04	11,11,14,18	0
2	SO4	A	3002	5/5	0.98	0.16	24,24,29,35	0
3	FAD	A	801	53/53	0.99	0.05	5,6,7,8	0
3	FAD	B	801	53/53	0.99	0.05	6,7,8,8	0

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 801:

$2mF_o-DF_c$ (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.