



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 09:44 pm BST

PDB ID : 3AYI
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 : Ida, K.; Suguro, M.; 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

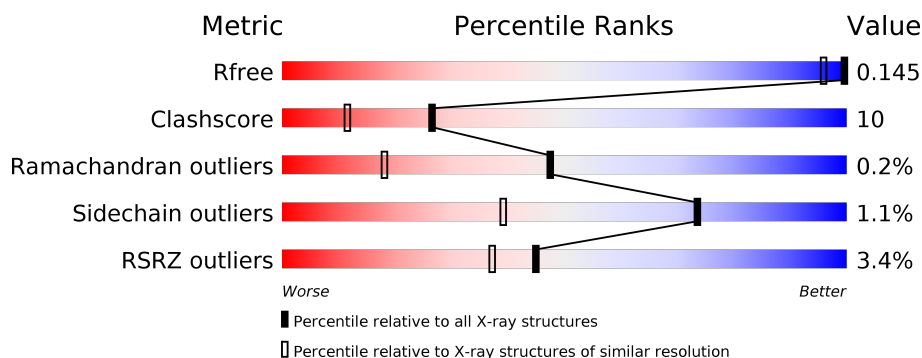
1 Overall quality at a glance

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>78%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	B	721	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>9%</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	B	3001	-	X	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12775 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.

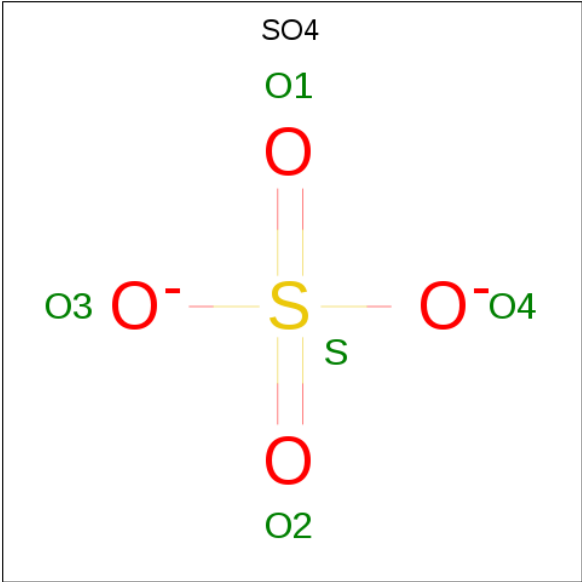
- Molecule 1 is a protein called Pro-enzyme of L-phenylalanine oxidase.

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	B	1	Total	O	S	0	0
			5	4	1		

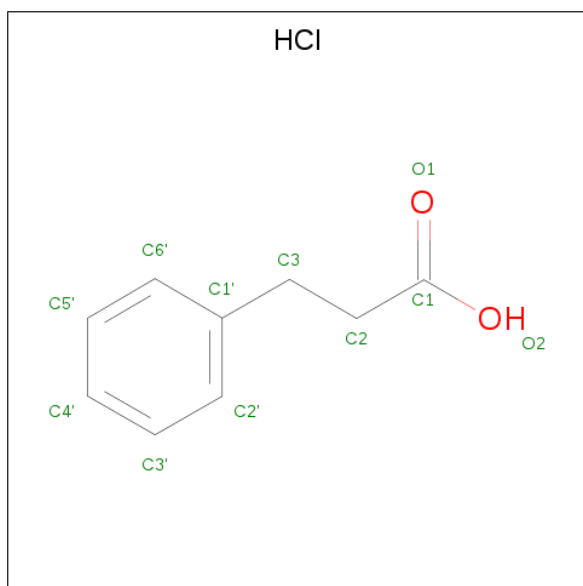
- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 4 is HYDROCINNAMIC ACID (three-letter code: HCI) (formula: $C_9H_{10}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	9	2		
4	B	1	Total	C	O	0	0
			11	9	2		

- 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		

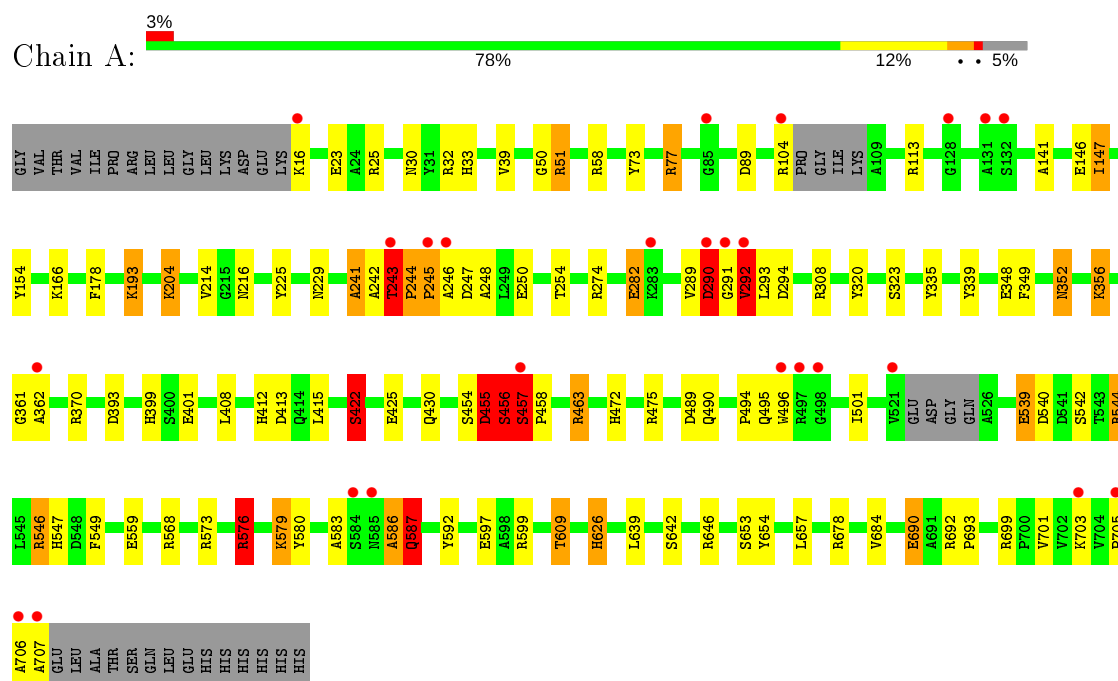
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1122	Total	O	0	0
			1122	1122		
6	B	1079	Total	O	0	0
			1079	1079		

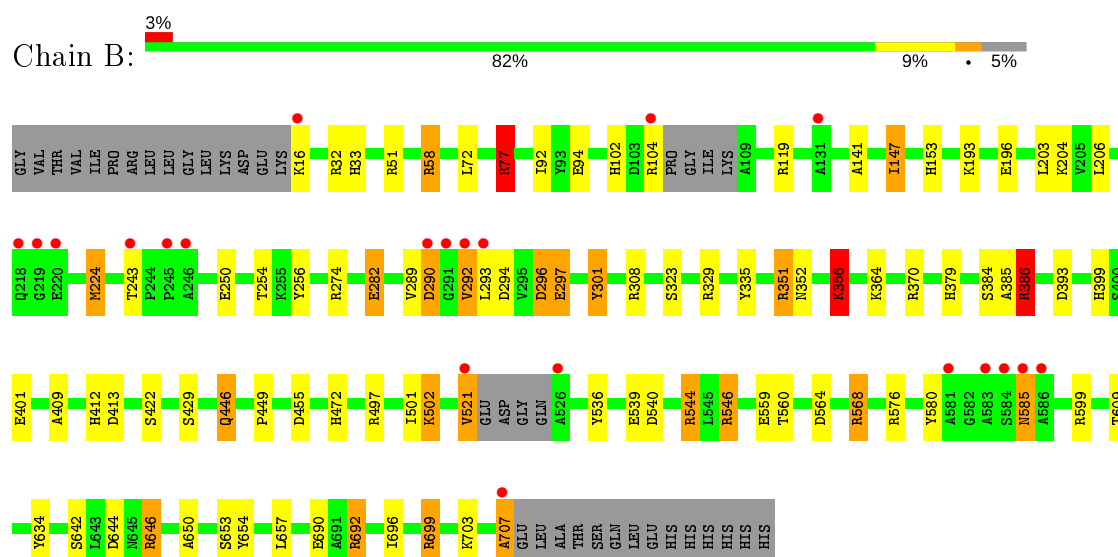
3 Residue-property plots [i](#)

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	101.29Å 112.69Å 136.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.56 – 1.25 36.31 – 1.25	Depositor EDS
% Data completeness (in resolution range)	97.1 (37.56-1.25) 97.1 (36.31-1.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 1.25Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.104 , 0.131 0.119 , 0.145	Depositor DCC
R_{free} test set	20896 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	11.0	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.6	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	0.98	EDS
Total number of atoms	12775	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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, HCl, 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	1.45	67/5347 (1.3%)	1.38	70/7300 (1.0%)
1	B	1.42	56/5347 (1.0%)	1.58	59/7300 (0.8%)
All	All	1.43	123/10694 (1.2%)	1.48	129/14600 (0.9%)

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	9
1	B	0	4
All	All	0	13

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	297	GLU	CD-OE2	22.89	1.50	1.25
1	B	282	GLU	CD-OE2	16.51	1.43	1.25
1	A	422	SER	CA-CB	16.16	1.77	1.52
1	B	386	ARG	CZ-NH1	13.56	1.50	1.33
1	B	58	ARG	CZ-NH2	13.01	1.50	1.33
1	B	576	ARG	CZ-NH2	12.36	1.49	1.33
1	B	282	GLU	CG-CD	12.32	1.70	1.51
1	A	609	THR	CB-CG2	-11.59	1.14	1.52
1	A	51	ARG	CG-CD	11.56	1.80	1.51
1	A	282	GLU	CD-OE2	11.42	1.38	1.25
1	B	544	ARG	CG-CD	11.38	1.80	1.51
1	A	245	PRO	N-CA	11.38	1.66	1.47
1	B	609	THR	CB-CG2	-11.19	1.15	1.52
1	B	147	ILE	CA-CB	10.72	1.79	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	559	GLU	CG-CD	10.59	1.67	1.51
1	B	301	TYR	CG-CD2	-10.54	1.25	1.39
1	A	323	SER	CA-CB	10.35	1.68	1.52
1	A	544	ARG	CD-NE	10.10	1.63	1.46
1	A	246	ALA	C-O	9.78	1.42	1.23
1	A	559	GLU	CD-OE2	9.39	1.35	1.25
1	A	51	ARG	CZ-NH2	9.28	1.45	1.33
1	A	58	ARG	CZ-NH1	9.18	1.45	1.33
1	B	58	ARG	CZ-NH1	9.00	1.44	1.33
1	A	323	SER	CB-OG	-8.81	1.30	1.42
1	A	290	ASP	CB-CG	8.79	1.70	1.51
1	A	642	SER	CB-OG	8.78	1.53	1.42
1	A	544	ARG	CG-CD	8.78	1.73	1.51
1	B	356	LYS	CE-NZ	8.75	1.71	1.49
1	A	579	LYS	CD-CE	8.65	1.72	1.51
1	A	576	ARG	CG-CD	8.30	1.72	1.51
1	A	250	GLU	CG-CD	-8.27	1.39	1.51
1	B	707	ALA	CA-CB	8.27	1.69	1.52
1	A	282	GLU	CG-CD	8.26	1.64	1.51
1	A	32	ARG	CG-CD	-8.03	1.31	1.51
1	B	544	ARG	CD-NE	7.92	1.59	1.46
1	A	77	ARG	CZ-NH2	-7.90	1.22	1.33
1	B	560	THR	CA-CB	7.88	1.73	1.53
1	B	642	SER	CB-OG	7.85	1.52	1.42
1	B	559	GLU	CD-OE1	-7.75	1.17	1.25
1	B	301	TYR	CE2-CZ	-7.69	1.28	1.38
1	A	559	GLU	CB-CG	-7.66	1.37	1.52
1	A	576	ARG	CB-CG	-7.65	1.31	1.52
1	B	296	ASP	CB-CG	7.55	1.67	1.51
1	B	568	ARG	CD-NE	-7.49	1.33	1.46
1	B	429	SER	CB-OG	-7.48	1.32	1.42
1	B	544	ARG	CZ-NH1	7.43	1.42	1.33
1	A	544	ARG	NE-CZ	-7.30	1.23	1.33
1	B	609	THR	CB-OG1	7.25	1.57	1.43
1	A	568	ARG	CD-NE	-7.23	1.34	1.46
1	B	77	ARG	CD-NE	-7.14	1.34	1.46
1	A	609	THR	CB-OG1	7.09	1.57	1.43
1	B	580	TYR	CZ-OH	-7.09	1.25	1.37
1	B	599	ARG	NE-CZ	7.04	1.42	1.33
1	B	196	GLU	CG-CD	-7.01	1.41	1.51
1	A	146	GLU	CD-OE1	-6.96	1.18	1.25
1	A	463	ARG	CB-CG	-6.94	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	LYS	CE-NZ	6.87	1.66	1.49
1	A	425	GLU	CD-OE1	-6.87	1.18	1.25
1	B	386	ARG	CZ-NH2	6.65	1.41	1.33
1	B	292	VAL	CB-CG1	6.64	1.66	1.52
1	A	587	GLN	CD-OE1	6.59	1.38	1.24
1	B	364	LYS	CE-NZ	-6.52	1.32	1.49
1	A	576	ARG	CZ-NH2	-6.47	1.24	1.33
1	B	364	LYS	CG-CD	-6.47	1.30	1.52
1	B	384	SER	CB-OG	-6.44	1.33	1.42
1	A	23	GLU	CD-OE1	-6.41	1.18	1.25
1	A	568	ARG	NE-CZ	6.33	1.41	1.33
1	B	692	ARG	CZ-NH2	-6.32	1.24	1.33
1	B	422	SER	CA-CB	6.26	1.62	1.52
1	A	356	LYS	CD-CE	6.22	1.66	1.51
1	B	32	ARG	CG-CD	-6.18	1.36	1.51
1	B	386	ARG	CG-CD	6.10	1.67	1.51
1	B	301	TYR	CG-CD1	6.08	1.47	1.39
1	B	560	THR	CB-CG2	-6.05	1.32	1.52
1	B	580	TYR	CE1-CZ	-6.01	1.30	1.38
1	A	245	PRO	CB-CG	5.94	1.79	1.50
1	A	352	ASN	CB-CG	-5.93	1.37	1.51
1	A	463	ARG	CG-CD	5.88	1.66	1.51
1	A	586	ALA	CA-C	5.88	1.68	1.52
1	B	642	SER	CA-CB	5.86	1.61	1.52
1	A	348	GLU	CB-CG	-5.75	1.41	1.52
1	B	356	LYS	CD-CE	5.75	1.65	1.51
1	B	559	GLU	CD-OE2	-5.74	1.19	1.25
1	A	370	ARG	CZ-NH2	-5.70	1.25	1.33
1	A	496	TRP	CG-CD1	5.70	1.44	1.36
1	B	323	SER	CA-CB	5.69	1.61	1.52
1	A	599	ARG	NE-CZ	5.68	1.40	1.33
1	A	684	VAL	CB-CG2	-5.68	1.41	1.52
1	B	546	ARG	CZ-NH2	-5.66	1.25	1.33
1	A	544	ARG	CZ-NH1	5.65	1.40	1.33
1	A	339	TYR	CE2-CZ	-5.64	1.31	1.38
1	A	214	VAL	CB-CG2	5.62	1.64	1.52
1	A	546	ARG	CG-CD	5.61	1.66	1.51
1	B	502	LYS	CG-CD	5.61	1.71	1.52
1	A	243	THR	CA-CB	5.58	1.67	1.53
1	B	224	MET	SD-CE	5.58	2.09	1.77
1	A	546	ARG	CD-NE	5.53	1.55	1.46
1	A	544	ARG	CZ-NH2	-5.51	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	446	GLN	CG-CD	5.49	1.63	1.51
1	B	634	TYR	CE1-CZ	-5.48	1.31	1.38
1	A	242	ALA	C-O	5.47	1.33	1.23
1	B	204	LYS	CD-CE	5.47	1.65	1.51
1	B	351	ARG	CG-CD	5.42	1.65	1.51
1	A	401	GLU	CD-OE1	-5.42	1.19	1.25
1	A	609	THR	CA-CB	5.41	1.67	1.53
1	A	147	ILE	CA-CB	5.41	1.67	1.54
1	A	282	GLU	CD-OE1	5.41	1.31	1.25
1	A	356	LYS	CE-NZ	5.36	1.62	1.49
1	B	204	LYS	CE-NZ	-5.35	1.35	1.49
1	B	297	GLU	CG-CD	5.29	1.59	1.51
1	A	568	ARG	CG-CD	-5.28	1.38	1.51
1	A	597	GLU	CD-OE2	-5.27	1.19	1.25
1	B	224	MET	CB-CG	-5.25	1.34	1.51
1	A	113	ARG	CD-NE	5.17	1.55	1.46
1	A	282	GLU	CB-CG	5.14	1.61	1.52
1	A	242	ALA	N-CA	5.11	1.56	1.46
1	B	576	ARG	CZ-NH1	-5.10	1.26	1.33
1	A	546	ARG	CZ-NH1	-5.09	1.26	1.33
1	A	580	TYR	CD2-CE2	5.04	1.47	1.39
1	B	609	THR	CA-CB	5.04	1.66	1.53
1	B	274	ARG	CZ-NH1	-5.03	1.26	1.33
1	A	154	TYR	CE1-CZ	-5.02	1.32	1.38
1	A	73	TYR	CG-CD1	-5.01	1.32	1.39

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	386	ARG	NE-CZ-NH2	-52.64	93.98	120.30
1	B	386	ARG	NE-CZ-NH1	32.54	136.57	120.30
1	B	576	ARG	NE-CZ-NH2	23.37	131.99	120.30
1	B	576	ARG	NE-CZ-NH1	-23.36	108.62	120.30
1	B	370	ARG	NE-CZ-NH2	-21.59	109.50	120.30
1	B	599	ARG	NE-CZ-NH1	20.54	130.57	120.30
1	B	646	ARG	NE-CZ-NH1	18.42	129.51	120.30
1	A	546	ARG	NE-CZ-NH1	15.98	128.29	120.30
1	A	576	ARG	NE-CZ-NH2	-14.76	112.92	120.30
1	B	351	ARG	NE-CZ-NH2	-14.68	112.96	120.30
1	B	370	ARG	NE-CZ-NH1	14.68	127.64	120.30
1	A	599	ARG	NE-CZ-NH1	14.62	127.61	120.30
1	B	77	ARG	NE-CZ-NH1	14.54	127.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	576	ARG	NE-CZ-NH1	14.43	127.52	120.30
1	A	77	ARG	NE-CZ-NH2	-14.27	113.16	120.30
1	A	51	ARG	NE-CZ-NH1	-14.19	113.20	120.30
1	A	77	ARG	NE-CZ-NH1	13.92	127.26	120.30
1	A	58	ARG	NE-CZ-NH1	13.57	127.08	120.30
1	A	455	ASP	CB-CG-OD1	-13.01	106.60	118.30
1	B	58	ARG	NE-CZ-NH1	-12.67	113.97	120.30
1	A	58	ARG	NE-CZ-NH2	-12.09	114.26	120.30
1	A	692	ARG	NE-CZ-NH2	-11.95	114.32	120.30
1	A	51	ARG	NE-CZ-NH2	11.86	126.23	120.30
1	B	351	ARG	NE-CZ-NH1	11.84	126.22	120.30
1	A	546	ARG	CD-NE-CZ	11.34	139.48	123.60
1	B	77	ARG	CD-NE-CZ	11.34	139.48	123.60
1	A	568	ARG	NE-CZ-NH1	10.93	125.77	120.30
1	B	646	ARG	NE-CZ-NH2	-10.89	114.85	120.30
1	B	568	ARG	NE-CZ-NH1	10.77	125.69	120.30
1	A	32	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	B	386	ARG	CD-NE-CZ	10.75	138.66	123.60
1	A	370	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	A	599	ARG	NE-CZ-NH2	-10.31	115.15	120.30
1	B	699	ARG	NE-CZ-NH2	-10.08	115.26	120.30
1	B	599	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	B	609	THR	OG1-CB-CG2	-9.77	87.54	110.00
1	A	204	LYS	CD-CE-NZ	9.75	134.13	111.70
1	A	544	ARG	NE-CZ-NH2	9.40	125.00	120.30
1	A	290	ASP	CB-CG-OD1	9.05	126.45	118.30
1	B	296	ASP	CB-CG-OD1	8.99	126.39	118.30
1	A	701	VAL	CG1-CB-CG2	8.96	125.23	110.90
1	B	692	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	B	386	ARG	NH1-CZ-NH2	8.84	129.12	119.40
1	A	51	ARG	CB-CG-CD	8.61	134.00	111.60
1	B	308	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	A	247	ASP	CB-CG-OD1	-8.52	110.63	118.30
1	A	457	SER	C-N-CD	8.50	146.26	128.40
1	B	77	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	B	308	ARG	NE-CZ-NH2	-8.31	116.15	120.30
1	A	609	THR	OG1-CB-CG2	-8.31	90.89	110.00
1	A	546	ARG	NH1-CZ-NH2	-8.27	110.30	119.40
1	B	692	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	A	678	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	B	544	ARG	CD-NE-CZ	-8.07	112.31	123.60
1	A	293	LEU	CB-CG-CD1	8.02	124.64	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	PRO	O-C-N	-7.94	110.00	122.70
1	A	89	ASP	CB-CG-OD1	7.90	125.41	118.30
1	B	297	GLU	CG-CD-OE1	-7.88	102.53	118.30
1	B	119	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	A	294	ASP	CB-CG-OD1	7.59	125.13	118.30
1	B	256	TYR	CZ-CE2-CD2	-7.35	113.18	119.80
1	B	297	GLU	CG-CD-OE2	7.35	133.00	118.30
1	A	457	SER	N-CA-C	7.33	130.79	111.00
1	B	644	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	B	256	TYR	CD1-CE1-CZ	-7.05	113.46	119.80
1	B	58	ARG	CA-CB-CG	-7.02	97.96	113.40
1	B	576	ARG	CD-NE-CZ	6.99	133.38	123.60
1	B	497	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	256	TYR	CE1-CZ-CE2	6.84	130.75	119.80
1	A	463	ARG	CG-CD-NE	-6.80	97.53	111.80
1	B	521	VAL	N-CA-C	-6.77	92.71	111.00
1	B	544	ARG	NE-CZ-NH2	6.77	123.68	120.30
1	A	349	PHE	CB-CG-CD1	6.75	125.53	120.80
1	B	203	LEU	CB-CG-CD1	6.73	122.44	111.00
1	A	245	PRO	CA-C-O	6.67	136.22	120.20
1	A	455	ASP	O-C-N	-6.64	112.07	122.70
1	A	539	GLU	OE1-CD-OE2	-6.56	115.43	123.30
1	A	592	TYR	CB-CG-CD2	6.56	124.94	121.00
1	A	692	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	A	690	GLU	OE1-CD-OE2	6.46	131.06	123.30
1	B	290	ASP	CB-CG-OD1	-6.45	112.50	118.30
1	A	546	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	A	626	HIS	CG-ND1-CE1	-6.42	97.35	105.70
1	B	568	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	B	282	GLU	CG-CD-OE2	6.41	131.11	118.30
1	A	241	ALA	O-C-N	-6.32	112.59	122.70
1	A	699	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	B	274	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	B	497	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	B	282	GLU	CG-CD-OE1	-6.13	106.05	118.30
1	A	32	ARG	NH1-CZ-NH2	-6.12	112.67	119.40
1	A	348	GLU	OE1-CD-OE2	-6.08	116.00	123.30
1	A	549	PHE	CB-CG-CD2	6.00	125.00	120.80
1	B	544	ARG	CG-CD-NE	5.97	124.33	111.80
1	A	225	TYR	CB-CG-CD2	5.96	124.58	121.00
1	B	580	TYR	CB-CG-CD1	5.93	124.56	121.00
1	A	544	ARG	CD-NE-CZ	-5.91	115.33	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	GLU	OE1-CD-OE2	5.89	130.37	123.30
1	A	422	SER	CA-CB-OG	-5.87	95.36	111.20
1	B	568	ARG	CG-CD-NE	-5.84	99.53	111.80
1	A	646	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	25	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	573	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	30	ASN	CB-CG-OD1	-5.72	110.17	121.60
1	A	544	ARG	CG-CD-NE	5.69	123.75	111.80
1	A	113	ARG	NE-CZ-NH2	5.69	123.14	120.30
1	A	457	SER	CB-CA-C	-5.67	99.32	110.10
1	A	456	SER	CB-CA-C	5.58	120.71	110.10
1	B	243	THR	CA-CB-CG2	-5.57	104.61	112.40
1	A	356	LYS	CD-CE-NZ	-5.51	99.02	111.70
1	B	384	SER	N-CA-CB	-5.43	102.36	110.50
1	A	489	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	690	GLU	OE1-CD-OE2	-5.40	116.82	123.30
1	A	308	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	699	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	422	SER	N-CA-CB	-5.37	102.45	110.50
1	B	501	ILE	CB-CG1-CD1	5.32	128.81	113.90
1	B	329	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	B	564	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	370	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	B	646	ARG	CD-NE-CZ	-5.22	116.28	123.60
1	A	320	TYR	CB-CG-CD1	5.21	124.13	121.00
1	B	77	ARG	CG-CD-NE	-5.17	100.93	111.80
1	A	489	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	A	568	ARG	NH1-CZ-NH2	-5.12	113.77	119.40
1	B	119	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	246	ALA	O-C-N	5.10	130.86	122.70
1	A	178	PHE	CB-CG-CD2	5.03	124.32	120.80
1	B	536	TYR	CB-CG-CD2	5.02	124.01	121.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	ALA	Mainchain
1	A	243	THR	Mainchain
1	A	244	PRO	Peptide
1	A	335	TYR	Sidechain
1	A	430	GLN	Sidechain

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Mol	Chain	Res	Type	Group
1	A	454	SER	Peptide
1	A	455	ASP	Mainchain
1	A	456	SER	Mainchain
1	A	654	TYR	Sidechain
1	B	335	TYR	Sidechain
1	B	385	ALA	Mainchain
1	B	654	TYR	Sidechain
1	B	77	ARG	Sidechain

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	5102	116	0
1	B	5212	0	5102	105	0
2	A	5	0	0	0	0
2	B	5	0	0	2	0
3	A	53	0	31	1	0
3	B	53	0	31	1	0
4	A	11	0	9	0	0
4	B	11	0	9	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	1122	0	0	68	9
6	B	1079	0	0	57	8
All	All	12775	0	10300	215	9

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 10.

All (215) 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:422:SER:CB	1:A:422:SER:CA	1.77	1.63
1:B:544:ARG:CD	1:B:544:ARG:CG	1.80	1.57
1:B:147:ILE:CB	1:B:147:ILE:CA	1.79	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ARG:CD	1:A:51:ARG:CG	1.80	1.54
1:B:356:LYS:NZ	1:B:356:LYS:CE	1.70	1.49
1:A:245:PRO:CG	1:A:245:PRO:CB	1.79	1.49
1:B:224:MET:SD	1:B:224:MET:CE	2.09	1.41
1:B:290:ASP:OD2	1:B:292:VAL:CG1	1.77	1.31
1:B:296:ASP:HB3	6:B:7102:HOH:O	1.10	1.27
1:B:352:ASN:HB3	6:B:7099:HOH:O	1.08	1.22
1:B:290:ASP:OD2	1:B:292:VAL:HG12	1.08	1.21
1:A:707:ALA:HA	6:A:7070:HOH:O	1.41	1.20
1:B:206:LEU:CD1	6:B:7170:HOH:O	1.89	1.17
1:A:456:SER:HA	6:A:7047:HOH:O	1.44	1.17
1:A:455:ASP:HB3	6:A:7072:HOH:O	1.43	1.15
1:A:576:ARG:NH1	6:A:7144:HOH:O	1.70	1.14
1:B:707:ALA:HB1	6:B:7109:HOH:O	1.44	1.14
1:A:495:GLN:NE2	6:A:7133:HOH:O	1.81	1.12
1:B:290:ASP:CG	1:B:292:VAL:HG12	1.71	1.10
1:B:58:ARG:HG2	6:B:7095:HOH:O	1.54	1.06
1:A:243:THR:HG22	6:A:6994:HOH:O	1.56	1.05
1:B:301:TYR:HE2	6:B:7017:HOH:O	1.41	1.04
1:A:707:ALA:CB	6:A:7117:HOH:O	2.03	1.03
1:B:206:LEU:HD22	6:B:7134:HOH:O	1.60	1.02
1:A:690:GLU:OE2	6:A:7121:HOH:O	1.79	1.01
1:B:51:ARG:NH2	6:B:7076:HOH:O	1.93	0.99
1:A:495:GLN:HG2	6:A:7133:HOH:O	1.63	0.97
1:B:521:VAL:HA	6:B:7052:HOH:O	1.63	0.97
1:B:206:LEU:HD11	6:B:7170:HOH:O	1.58	0.97
6:A:7194:HOH:O	1:B:301:TYR:CE1	2.17	0.97
1:A:282:GLU:HG3	6:A:6114:HOH:O	1.62	0.96
1:B:282:GLU:HG3	6:B:5901:HOH:O	1.63	0.96
1:B:301:TYR:CE2	6:B:7017:HOH:O	2.18	0.93
1:B:51:ARG:NH1	6:B:7076:HOH:O	2.00	0.93
1:B:58:ARG:CG	6:B:7095:HOH:O	2.14	0.92
1:B:206:LEU:CD2	6:B:7134:HOH:O	2.15	0.91
1:A:243:THR:CG2	6:A:6994:HOH:O	2.12	0.91
1:A:290:ASP:O	6:A:7180:HOH:O	1.88	0.91
1:B:379:HIS:HE1	1:B:646:ARG:H	1.17	0.89
1:B:546:ARG:NH1	2:B:3001:SO4:O3	2.06	0.89
1:B:51:ARG:CZ	6:B:7076:HOH:O	2.19	0.88
1:B:104:ARG:HA	6:B:7038:HOH:O	1.73	0.88
1:B:206:LEU:HD13	6:B:7170:HOH:O	1.58	0.87
1:A:707:ALA:HB1	6:A:5368:HOH:O	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ARG:CA	6:B:7038:HOH:O	2.25	0.84
1:A:77:ARG:HD2	6:A:6253:HOH:O	1.77	0.83
1:B:351:ARG:NH2	6:B:6363:HOH:O	1.87	0.83
1:A:254:THR:HG22	6:A:5991:HOH:O	1.78	0.82
1:A:707:ALA:HA	6:A:7117:HOH:O	1.80	0.81
1:B:521:VAL:CA	6:B:7052:HOH:O	2.22	0.81
1:A:216:ASN:ND2	6:A:6452:HOH:O	2.13	0.80
1:B:707:ALA:O	6:B:7141:HOH:O	2.00	0.79
1:A:587:GLN:NE2	1:A:587:GLN:HA	1.99	0.78
1:A:490:GLN:NE2	6:A:7190:HOH:O	2.16	0.78
1:A:422:SER:HB3	6:A:5644:HOH:O	1.83	0.77
1:B:297:GLU:OE1	6:B:7185:HOH:O	2.03	0.77
1:B:206:LEU:CB	6:B:7134:HOH:O	2.32	0.77
1:B:707:ALA:CB	6:B:7109:HOH:O	2.16	0.76
1:A:413:ASP:HB3	6:A:7124:HOH:O	1.84	0.76
1:A:495:GLN:CD	6:A:7133:HOH:O	2.18	0.76
1:A:587:GLN:HE21	1:A:587:GLN:HA	1.50	0.76
1:B:401:GLU:OE2	6:B:6343:HOH:O	2.04	0.76
1:A:576:ARG:NH2	6:A:6997:HOH:O	1.82	0.76
1:A:422:SER:OG	1:A:422:SER:CA	2.33	0.75
1:B:206:LEU:HB2	6:B:7134:HOH:O	1.87	0.75
1:A:456:SER:CA	6:A:7047:HOH:O	2.17	0.74
6:A:6582:HOH:O	1:B:301:TYR:CE1	2.41	0.74
1:A:193:LYS:CE	6:A:7073:HOH:O	2.34	0.74
1:A:245:PRO:HA	6:A:7110:HOH:O	1.87	0.74
1:B:224:MET:HB2	1:B:224:MET:CE	2.18	0.74
1:A:290:ASP:HB3	1:A:292:VAL:CG1	2.18	0.73
1:B:472:HIS:HE1	1:B:539:GLU:OE2	1.70	0.73
1:A:579:LYS:NZ	6:A:6593:HOH:O	2.19	0.73
1:B:546:ARG:NH1	2:B:3001:SO4:S	2.62	0.73
1:B:544:ARG:HD2	6:B:5651:HOH:O	1.88	0.72
1:B:293:LEU:O	6:B:7155:HOH:O	2.05	0.72
1:A:544:ARG:NH1	6:A:5785:HOH:O	2.23	0.72
1:A:540:ASP:OD2	1:B:472:HIS:HD2	1.72	0.72
1:A:472:HIS:HD2	1:B:540:ASP:OD2	1.72	0.72
1:B:147:ILE:CA	1:B:147:ILE:CG1	2.66	0.72
1:A:706:ALA:O	1:A:707:ALA:HB2	1.89	0.71
1:B:290:ASP:N	1:B:290:ASP:OD1	2.19	0.71
1:A:707:ALA:CA	6:A:7117:HOH:O	2.29	0.71
1:A:472:HIS:HE1	1:A:539:GLU:OE2	1.73	0.70
1:A:422:SER:CB	1:A:422:SER:N	2.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:ARG:NH2	1:A:609:THR:OG1	2.25	0.69
1:B:250:GLU:OE2	1:B:254:THR:HG21	1.93	0.69
1:B:193:LYS:HD2	6:B:7098:HOH:O	1.93	0.69
1:A:193:LYS:CD	6:A:7073:HOH:O	2.42	0.68
1:A:193:LYS:HD2	6:A:5814:HOH:O	1.92	0.68
1:B:386:ARG:HG2	6:B:7103:HOH:O	1.93	0.68
1:A:707:ALA:HB1	6:A:7117:HOH:O	1.78	0.68
1:B:77:ARG:HD3	6:B:5379:HOH:O	1.94	0.68
1:A:457:SER:OG	1:B:292:VAL:HG11	1.95	0.67
1:A:544:ARG:HD2	6:A:5807:HOH:O	1.94	0.67
1:B:393:ASP:OD2	1:B:399:HIS:HE1	1.78	0.67
1:A:412:HIS:HD2	1:A:653:SER:OG	1.78	0.67
1:B:544:ARG:NH1	6:B:7069:HOH:O	2.27	0.67
6:A:6661:HOH:O	1:B:293:LEU:HD23	1.96	0.66
1:A:413:ASP:HB3	6:B:6849:HOH:O	1.94	0.66
1:A:290:ASP:HB3	1:A:292:VAL:HG11	1.78	0.65
1:A:290:ASP:OD2	6:A:7100:HOH:O	2.14	0.65
1:B:290:ASP:OD2	1:B:292:VAL:HG11	1.92	0.65
1:A:352:ASN:OD1	6:A:6914:HOH:O	2.14	0.64
1:A:626:HIS:HE1	6:A:5461:HOH:O	1.79	0.64
1:A:16:LYS:N	6:A:6192:HOH:O	2.30	0.64
1:A:361:GLY:HA3	6:A:5906:HOH:O	1.98	0.64
1:A:586:ALA:O	1:A:587:GLN:NE2	2.31	0.64
1:A:413:ASP:CB	6:A:7124:HOH:O	2.43	0.63
1:A:705:PRO:HG3	6:A:5518:HOH:O	1.97	0.63
6:A:7194:HOH:O	1:B:301:TYR:HE1	1.69	0.63
1:B:568:ARG:CZ	6:B:7179:HOH:O	2.47	0.63
1:B:104:ARG:C	6:B:7038:HOH:O	2.36	0.62
1:B:379:HIS:CE1	1:B:646:ARG:H	2.08	0.62
1:B:412:HIS:HD2	1:B:653:SER:OG	1.83	0.62
1:A:542:SER:OG	1:A:546:ARG:NH2	2.32	0.62
1:B:147:ILE:CA	1:B:147:ILE:HD13	2.29	0.62
1:A:289:VAL:C	1:A:291:GLY:H	2.04	0.61
1:A:245:PRO:HB2	1:A:248:ALA:HB2	1.82	0.61
1:A:463:ARG:HG2	6:B:7185:HOH:O	1.99	0.61
1:B:102:HIS:HD2	6:B:5646:HOH:O	1.82	0.61
1:B:289:VAL:HB	1:B:293:LEU:HD12	1.82	0.60
1:A:576:ARG:NH1	6:A:6997:HOH:O	2.34	0.60
1:B:544:ARG:CD	1:B:544:ARG:CB	2.77	0.60
1:A:587:GLN:CA	1:A:587:GLN:NE2	2.65	0.59
1:A:51:ARG:NE	1:A:51:ARG:CG	2.64	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:ALA:O	1:A:707:ALA:CB	2.51	0.59
1:A:290:ASP:CB	1:A:292:VAL:CG1	2.81	0.58
1:B:224:MET:CE	1:B:224:MET:CG	2.81	0.58
1:B:254:THR:HG22	6:B:6518:HOH:O	2.04	0.58
1:A:422:SER:CB	1:A:422:SER:C	2.69	0.58
1:B:153:HIS:HE1	6:B:5277:HOH:O	1.85	0.58
1:A:547:HIS:HE1	6:B:6248:HOH:O	1.85	0.57
1:A:639:LEU:O	1:A:707:ALA:HB3	2.04	0.57
1:A:147:ILE:HG22	1:A:147:ILE:O	2.05	0.57
1:A:245:PRO:HB2	1:A:248:ALA:CB	2.33	0.57
1:B:147:ILE:HD13	1:B:147:ILE:HA	1.87	0.57
1:B:147:ILE:CA	1:B:147:ILE:CD1	2.82	0.57
1:A:193:LYS:N	1:A:193:LYS:HD3	2.19	0.56
1:A:393:ASP:OD2	1:A:399:HIS:HE1	1.87	0.56
1:A:362:ALA:O	6:A:6698:HOH:O	2.18	0.56
1:A:243:THR:CG2	6:A:5583:HOH:O	2.53	0.56
1:A:229:ASN:HB3	6:A:7125:HOH:O	2.05	0.56
1:B:141:ALA:HA	3:B:801:FAD:C4X	2.36	0.56
1:A:361:GLY:CA	6:A:5906:HOH:O	2.52	0.55
6:A:7194:HOH:O	1:B:301:TYR:CD1	2.50	0.55
6:A:7101:HOH:O	1:B:413:ASP:HB3	2.06	0.55
1:A:361:GLY:C	6:A:5906:HOH:O	2.45	0.55
1:A:457:SER:O	1:A:458:PRO:C	2.43	0.54
1:A:243:THR:HG21	6:A:5583:HOH:O	2.06	0.54
1:A:245:PRO:HB2	1:A:248:ALA:H	1.72	0.54
1:A:626:HIS:CD2	6:A:5817:HOH:O	2.61	0.54
1:A:455:ASP:CB	6:A:7072:HOH:O	2.24	0.54
1:B:147:ILE:CB	1:B:147:ILE:N	2.63	0.54
1:A:495:GLN:CG	6:A:7133:HOH:O	2.24	0.53
1:A:289:VAL:C	1:A:291:GLY:N	2.61	0.53
1:B:699:ARG:NH2	6:B:6900:HOH:O	2.27	0.53
1:B:646:ARG:NH1	6:B:7103:HOH:O	2.41	0.53
1:B:224:MET:CB	1:B:224:MET:CE	2.88	0.52
1:B:290:ASP:C	1:B:290:ASP:OD1	2.45	0.52
1:A:463:ARG:CG	6:B:7185:HOH:O	2.56	0.51
1:B:33:HIS:CE1	1:B:657:LEU:HD11	2.44	0.51
1:A:703:LYS:HD3	1:B:292:VAL:O	2.10	0.51
1:B:72:LEU:HD22	1:B:92:ILE:HD11	1.93	0.50
1:A:290:ASP:C	1:A:292:VAL:HG12	2.31	0.50
1:B:585:ASN:OD1	1:B:585:ASN:N	2.43	0.50
1:B:521:VAL:O	6:B:7052:HOH:O	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:MET:HB2	1:B:224:MET:HE2	1.91	0.49
1:A:626:HIS:HD2	6:B:7102:HOH:O	1.95	0.49
1:A:141:ALA:HA	3:A:801:FAD:C4X	2.42	0.49
1:B:147:ILE:CA	1:B:147:ILE:CG2	2.81	0.49
1:A:455:ASP:CA	6:A:7072:HOH:O	2.59	0.49
1:A:289:VAL:O	1:A:291:GLY:N	2.46	0.49
1:A:33:HIS:CE1	1:A:657:LEU:HD11	2.48	0.49
1:A:703:LYS:HB3	1:A:703:LYS:HZ2	1.79	0.48
1:A:193:LYS:HD3	6:A:7073:HOH:O	2.10	0.48
1:A:494:PRO:HG2	1:A:501:ILE:HD12	1.95	0.48
1:A:50:GLY:O	1:A:51:ARG:NH1	2.47	0.47
1:A:576:ARG:HD3	6:A:5589:HOH:O	2.13	0.47
1:B:282:GLU:CG	6:B:5901:HOH:O	2.37	0.47
1:A:193:LYS:NZ	6:A:7073:HOH:O	2.40	0.47
6:A:6582:HOH:O	1:B:301:TYR:CD1	2.64	0.47
1:A:274:ARG:HB2	6:A:5378:HOH:O	2.15	0.47
1:A:422:SER:HB2	6:A:7106:HOH:O	2.13	0.47
1:A:457:SER:HG	1:B:292:VAL:HG11	1.79	0.47
1:A:408:LEU:HD13	1:A:415:LEU:HD11	1.97	0.46
1:B:94:GLU:O	1:B:102:HIS:HE1	1.98	0.46
1:A:639:LEU:O	1:A:707:ALA:CB	2.64	0.45
1:A:579:LYS:HE3	1:A:583:ALA:O	2.16	0.45
1:B:297:GLU:CG	6:B:7185:HOH:O	2.65	0.45
1:B:446:GLN:NE2	6:B:7151:HOH:O	2.35	0.45
1:B:455:ASP:OD2	6:B:7122:HOH:O	2.21	0.45
1:A:290:ASP:O	1:A:292:VAL:HG12	2.18	0.44
1:A:356:LYS:HD3	6:A:6061:HOH:O	2.17	0.44
1:A:707:ALA:HB2	6:A:7117:HOH:O	1.97	0.44
1:A:204:LYS:HB2	1:A:204:LYS:HE2	1.34	0.43
1:A:626:HIS:CE1	6:A:5461:HOH:O	2.62	0.43
1:A:703:LYS:NZ	6:A:6861:HOH:O	2.42	0.43
1:B:147:ILE:CB	1:B:147:ILE:C	2.74	0.43
1:A:703:LYS:HD2	1:B:294:ASP:HB3	2.00	0.42
1:B:585:ASN:CG	6:B:6548:HOH:O	2.57	0.42
1:B:696:ILE:HD11	6:B:6190:HOH:O	2.17	0.42
1:B:297:GLU:HG3	6:B:7185:HOH:O	2.18	0.42
1:B:692:ARG:NH1	6:B:7111:HOH:O	2.43	0.42
1:B:193:LYS:CD	6:B:7098:HOH:O	2.61	0.42
1:A:39:VAL:HB	1:A:693:PRO:HB2	2.02	0.42
1:B:224:MET:O	1:B:224:MET:HG3	2.18	0.42
1:A:166:LYS:HE3	6:A:6300:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:HIS:HD2	1:B:449:PRO:O	2.03	0.41
1:A:412:HIS:CD2	1:A:653:SER:OG	2.67	0.41
1:B:703:LYS:HD3	1:B:703:LYS:HA	1.94	0.41
1:B:77:ARG:CD	6:B:5379:HOH:O	2.60	0.40
1:A:244:PRO:O	6:A:7025:HOH:O	2.22	0.40
1:B:502:LYS:NZ	6:B:6890:HOH:O	2.17	0.40
1:B:409:ALA:HA	1:B:650:ALA:O	2.22	0.40

All (9) 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:5813:HOH:O	6:B:7087:HOH:O[2_665]	1.68	0.52
6:A:5499:HOH:O	6:B:7113:HOH:O[3_756]	1.72	0.48
6:A:6587:HOH:O	6:B:6992:HOH:O[2_664]	1.93	0.27
6:A:6068:HOH:O	6:B:7077:HOH:O[4_556]	1.95	0.25
6:A:6587:HOH:O	6:B:6273:HOH:O[2_664]	2.04	0.16
6:A:6985:HOH:O	6:B:5941:HOH:O[3_756]	2.09	0.11
6:A:6030:HOH:O	6:A:7060:HOH:O[3_746]	2.15	0.05
6:A:7004:HOH:O	6:B:6563:HOH:O[3_756]	2.17	0.03
6:A:5525:HOH:O	6:B:5533:HOH:O[4_556]	2.17	0.03

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	678/721 (94%)	661 (98%)	14 (2%)	3 (0%)	34 10
1	B	678/721 (94%)	666 (98%)	12 (2%)	0	100 100
All	All	1356/1442 (94%)	1327 (98%)	26 (2%)	3 (0%)	47 18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	ASP
1	A	292	VAL
1	A	457	SER

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%)	526 (98%)	8 (2%)	65	28
1	B	534/566 (94%)	530 (99%)	4 (1%)	84	57
All	All	1068/1132 (94%)	1056 (99%)	12 (1%)	73	39

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ARG
1	A	193	LYS
1	A	292	VAL
1	A	422	SER
1	A	457	SER
1	A	475	ARG
1	A	576	ARG
1	A	587	GLN
1	B	16	LYS
1	B	356	LYS
1	B	386	ARG
1	B	585	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	170	ASN
1	A	399	HIS
1	A	412	HIS

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Mol	Chain	Res	Type
1	A	472	HIS
1	A	547	HIS
1	A	587	GLN
1	A	626	HIS
1	B	102	HIS
1	B	153	HIS
1	B	379	HIS
1	B	399	HIS
1	B	412	HIS
1	B	446	GLN
1	B	472	HIS
1	B	547	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	$\# Z > 2$
2	SO4	B	3001	-	4,4,4	2.42	1 (25%)	6,6,6	4.76	6 (100%)
5	GOL	B	1902	-	5,5,5	0.95	0	5,5,5	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	B	801	-	51,58,58	1.32	3 (5%)	60,89,89	2.03	13 (21%)
2	SO4	A	3002	-	4,4,4	1.67	1 (25%)	6,6,6	3.28	2 (33%)
5	GOL	A	902	-	5,5,5	1.42	0	5,5,5	0.59	0
4	HCI	A	907	-	8,11,11	0.87	0	10,13,13	1.13	1 (10%)
3	FAD	A	801	-	51,58,58	1.15	4 (7%)	60,89,89	2.24	7 (11%)
4	HCI	B	1907	-	8,11,11	0.71	0	10,13,13	0.67	0

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
5	GOL	B	1902	-	-	0/4/4/4	-
3	FAD	B	801	-	-	3/30/50/50	0/6/6/6
5	GOL	A	902	-	-	0/4/4/4	-
4	HCI	A	907	-	-	0/3/5/5	0/1/1/1
3	FAD	A	801	-	-	5/30/50/50	0/6/6/6
4	HCI	B	1907	-	-	0/3/5/5	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	FAD	O4B-C1B	5.21	1.48	1.41
2	B	3001	SO4	O1-S	-4.28	1.22	1.46
3	B	801	FAD	C4-N3	3.43	1.39	1.33
3	A	801	FAD	C4-N3	3.03	1.38	1.33
3	A	801	FAD	C4X-N5	2.88	1.37	1.33
2	A	3002	SO4	O2-S	-2.53	1.32	1.46
3	A	801	FAD	C7M-C7	2.47	1.56	1.51
3	B	801	FAD	C6-C5X	-2.40	1.38	1.41
3	A	801	FAD	O4B-C1B	2.18	1.44	1.41

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	FAD	C4-N3-C2	13.39	126.45	115.14
2	B	3001	SO4	O4-S-O1	-6.86	73.49	109.31
3	B	801	FAD	C4-C4X-C10	-6.49	115.66	119.95
3	B	801	FAD	C4-N3-C2	6.34	120.50	115.14
2	B	3001	SO4	O4-S-O3	6.27	135.82	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3002	SO4	O3-S-O2	-5.95	78.24	109.31
3	A	801	FAD	C4X-C4-N3	-5.90	115.37	123.43
2	A	3002	SO4	O2-S-O1	5.11	147.14	109.43
2	B	3001	SO4	O3-S-O1	-5.00	83.24	109.31
3	B	801	FAD	C4X-N5-C5X	4.99	121.75	116.77
3	B	801	FAD	C1'-N10-C9A	4.98	122.22	118.29
3	B	801	FAD	C4-C4X-N5	4.17	123.36	118.60
3	A	801	FAD	C1'-N10-C9A	3.96	121.41	118.29
2	B	3001	SO4	O3-S-O2	3.54	127.77	109.31
3	B	801	FAD	C5'-C4'-C3'	-3.29	105.85	112.20
3	A	801	FAD	C5'-C4'-C3'	-2.89	106.62	112.20
3	B	801	FAD	O4B-C1B-C2B	-2.78	102.86	106.93
2	B	3001	SO4	O4-S-O2	-2.55	95.98	109.31
3	A	801	FAD	C4X-C10-N10	-2.51	117.72	120.30
3	B	801	FAD	C9A-C5X-N5	-2.49	118.46	122.36
3	B	801	FAD	C9-C9A-C5X	-2.46	115.68	119.88
4	A	907	HCI	C6'-C1'-C2'	2.31	121.80	118.17
2	B	3001	SO4	O2-S-O1	2.31	126.48	109.43
3	B	801	FAD	O4B-C4B-C3B	2.22	109.50	105.11
3	B	801	FAD	C4X-C4-N3	-2.19	120.44	123.43
3	B	801	FAD	O3'-C3'-C4'	-2.07	103.82	108.81
3	B	801	FAD	C6-C7-C8	-2.03	116.48	119.91
3	A	801	FAD	O2P-P-O1P	2.02	122.22	112.24
3	A	801	FAD	O4B-C1B-C2B	-2.01	104.00	106.93

There are no chirality outliers.

All (8) torsion outliers are listed below:

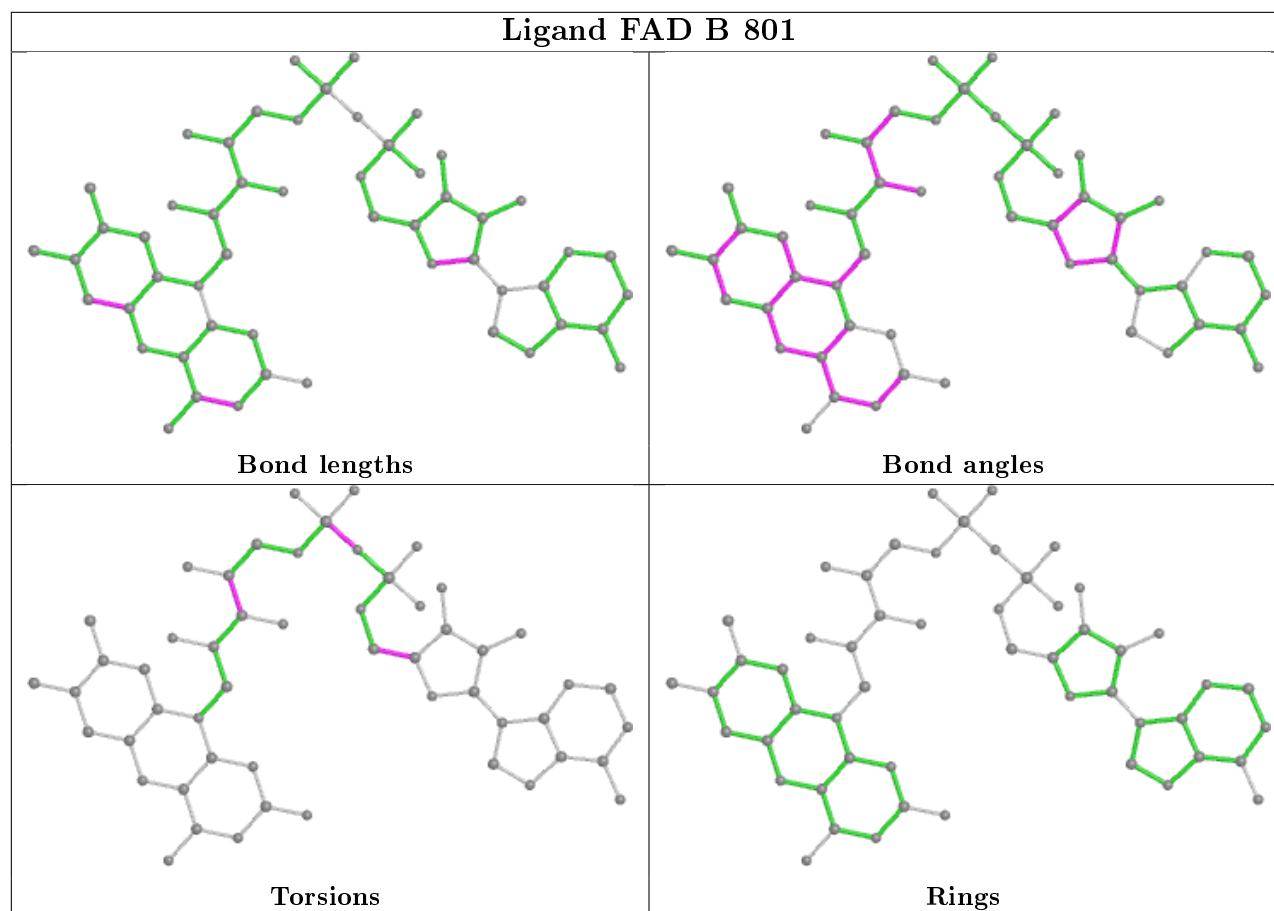
Mol	Chain	Res	Type	Atoms
3	B	801	FAD	PA-O3P-P-O5'
3	A	801	FAD	PA-O3P-P-O5'
3	A	801	FAD	C2'-C3'-C4'-O4'
3	A	801	FAD	C2'-C3'-C4'-C5'
3	A	801	FAD	O3'-C3'-C4'-C5'
3	A	801	FAD	O4B-C4B-C5B-O5B
3	B	801	FAD	O3'-C3'-C4'-C5'
3	B	801	FAD	O4B-C4B-C5B-O5B

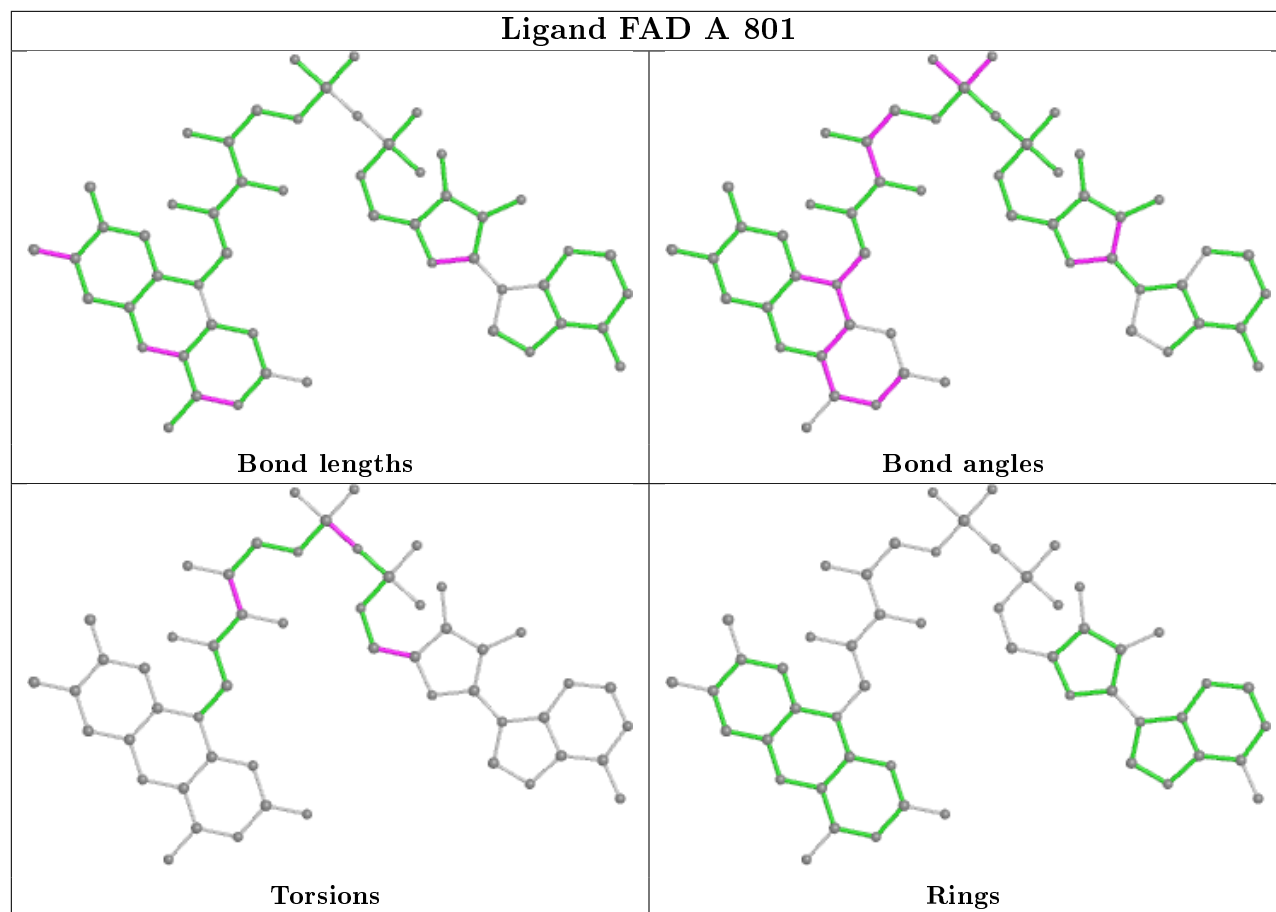
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3001	SO4	2	0
3	B	801	FAD	1	0
3	A	801	FAD	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	-0.31	25 (3%) 41 34	7, 12, 26, 46	0
1	B	684/721 (94%)	-0.29	21 (3%) 49 41	8, 13, 27, 41	0
All	All	1368/1442 (94%)	-0.30	46 (3%) 45 37	7, 13, 27, 46	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	293	LEU	8.1
1	A	707	ALA	7.8
1	A	362	ALA	7.2
1	B	707	ALA	7.1
1	B	521	VAL	6.5
1	B	585	ASN	6.2
1	A	521	VAL	6.0
1	A	104	ARG	5.9
1	A	292	VAL	5.6
1	B	292	VAL	5.4
1	A	496	TRP	5.1
1	A	498	GLY	4.5
1	A	246	ALA	4.2
1	A	497	ARG	3.6
1	B	218	GLN	3.6
1	B	104	ARG	3.6
1	A	16	LYS	3.4
1	B	246	ALA	3.3
1	B	583	ALA	3.3
1	B	290	ASP	3.3
1	A	291	GLY	3.3
1	B	16	LYS	3.3
1	A	706	ALA	3.2
1	B	584	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	131	ALA	3.2
1	B	243	THR	3.1
1	A	584	SER	3.0
1	A	132	SER	2.9
1	A	245	PRO	2.9
1	B	526	ALA	2.8
1	A	128	GLY	2.8
1	A	457	SER	2.8
1	A	85	GLY	2.6
1	A	703	LYS	2.5
1	B	219	GLY	2.5
1	A	585	ASN	2.5
1	B	131	ALA	2.5
1	A	243	THR	2.4
1	A	283	LYS	2.3
1	B	586	ALA	2.3
1	B	220	GLU	2.2
1	A	290	ASP	2.2
1	B	581	ALA	2.2
1	A	705	PRO	2.2
1	B	291	GLY	2.0
1	B	245	PRO	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	B	3001	5/5	0.95	0.12	22,25,29,39	0

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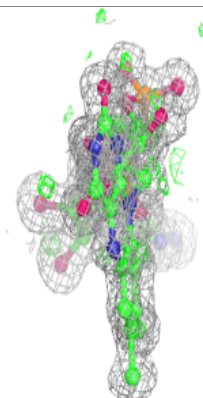
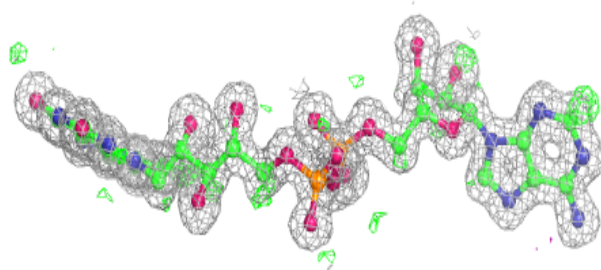
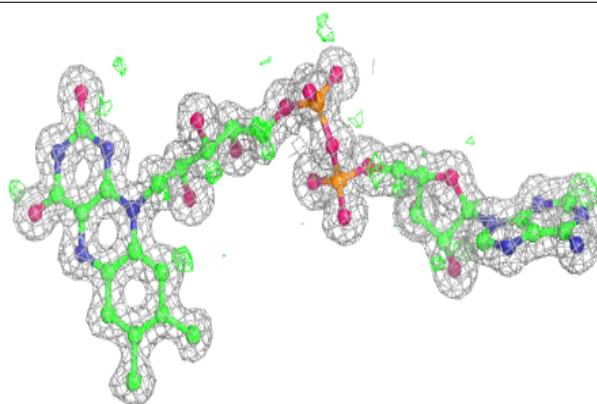
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	B	1902	6/6	0.97	0.07	14,15,17,20	0
2	SO4	A	3002	5/5	0.97	0.15	24,25,28,36	0
5	GOL	A	902	6/6	0.98	0.06	14,15,19,24	0
4	HCI	A	907	11/11	0.98	0.06	8,9,10,10	0
4	HCI	B	1907	11/11	0.98	0.09	9,9,11,12	0
3	FAD	A	801	53/53	0.99	0.05	7,8,9,10	0
3	FAD	B	801	53/53	0.99	0.06	7,8,9,10	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.

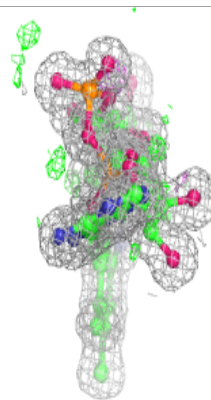
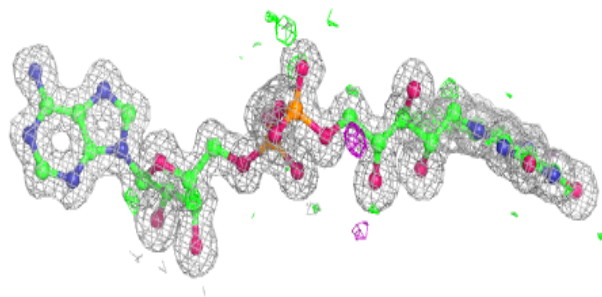
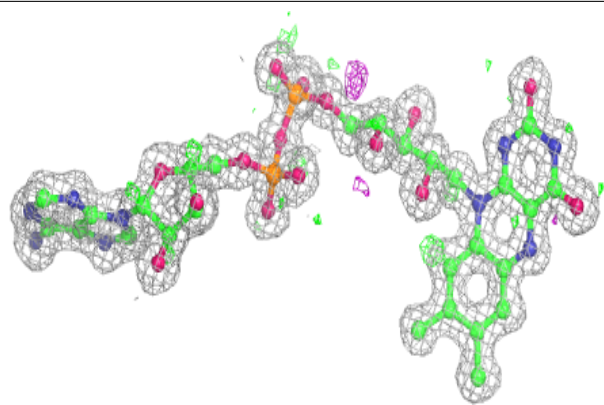
Electron density around FAD A 801:

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 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.