



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:47 am BST

PDB ID : 2YR5
Title : Crystal structure of L-phenylalanine oxidase from Psuedomonas sp.P501
Authors : Ida, K.; Kurabayashi, M.; Suguro, M.; Hikima, T.; Yamamoto, M.; Suzuki, H.
Deposited on : 2007-04-02
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

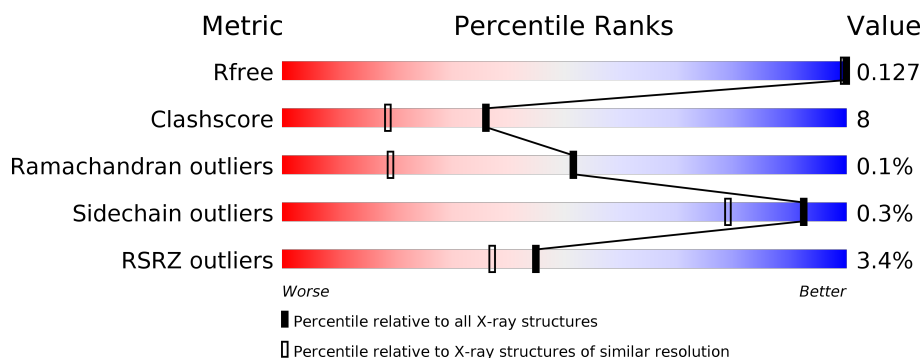
1 Overall quality at a glance

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>80%</div> <div>11%</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	SO4	A	3002	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12783 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.

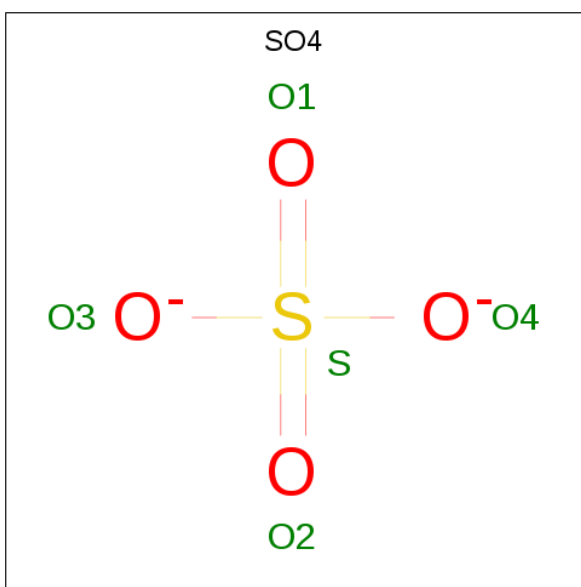
- Molecule 1 is a protein called Pro-enzyme of L-phenylalanine oxidase.

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:

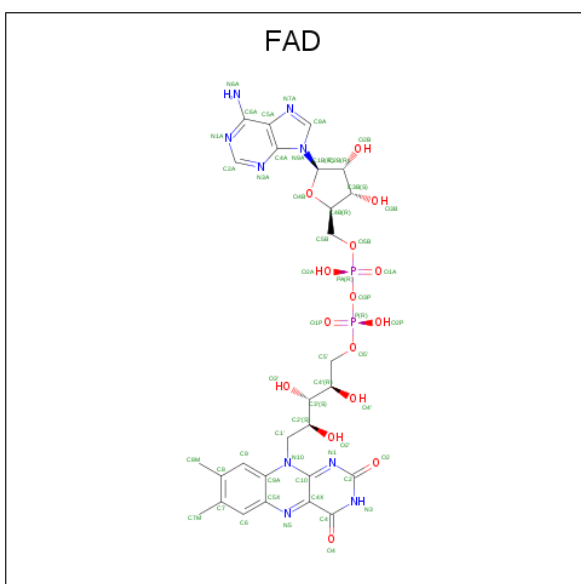
Chain	Residue	Modelled	Actual	Comment	Reference
A	714	LEU	-	EXPRESSION TAG	UNP Q5W9R9
A	715	GLU	-	EXPRESSION TAG	UNP Q5W9R9
A	716	HIS	-	EXPRESSION TAG	UNP Q5W9R9
A	717	HIS	-	EXPRESSION TAG	UNP Q5W9R9
A	718	HIS	-	EXPRESSION TAG	UNP Q5W9R9
A	719	HIS	-	EXPRESSION TAG	UNP Q5W9R9
A	720	HIS	-	EXPRESSION TAG	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 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

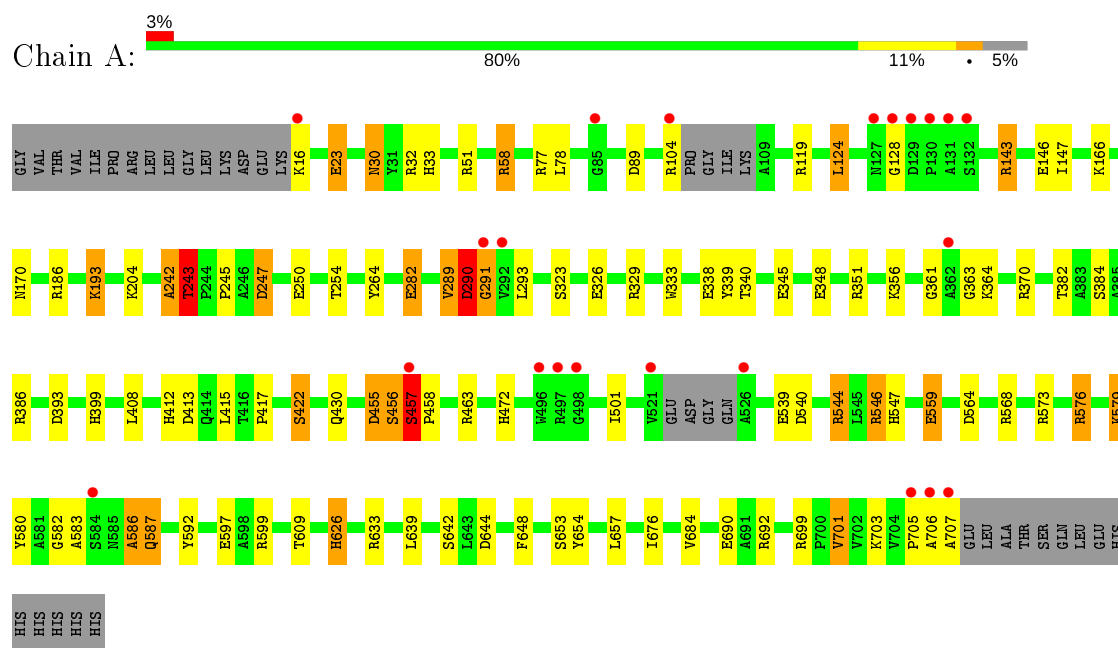
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1100	Total	O	0	0
			1100	1100		
5	B	1109	Total	O	0	0
			1109	1109		

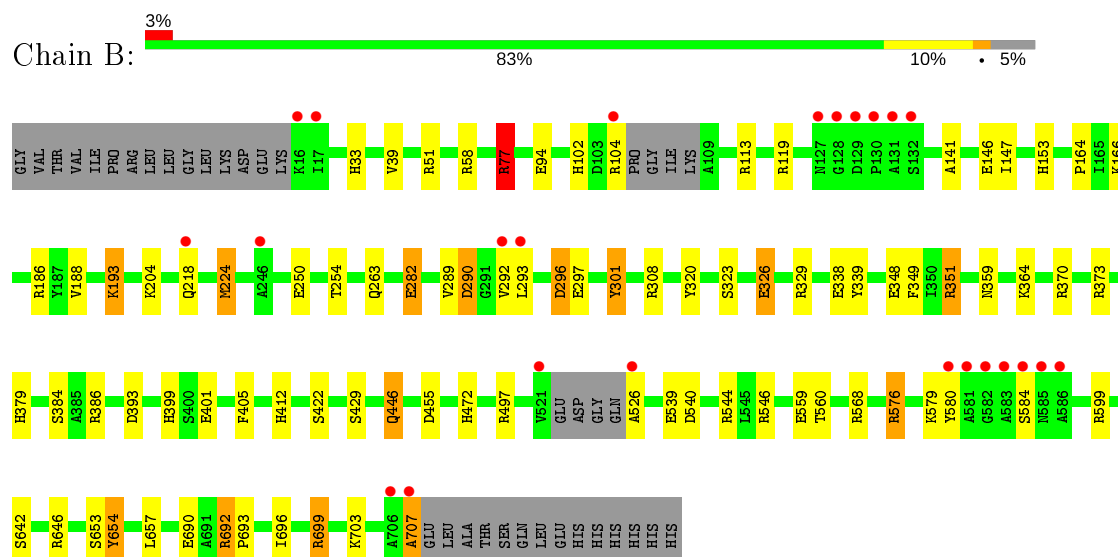
3 Residue-property plots [i](#)

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	101.65Å 112.62Å 136.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.62 – 1.25 47.63 – 1.25	Depositor EDS
% Data completeness (in resolution range)	97.8 (47.62-1.25) 97.8 (47.63-1.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 1.25Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.101 , 0.129 0.102 , 0.127	Depositor DCC
R_{free} test set	21030 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	9.5	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.1	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	12783	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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	1.42	62/5347 (1.2%)	1.30	59/7300 (0.8%)
1	B	1.34	40/5347 (0.7%)	1.30	50/7300 (0.7%)
All	All	1.38	102/10694 (1.0%)	1.30	109/14600 (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	2
All	All	0	7

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	297	GLU	CD-OE2	24.07	1.52	1.25
1	B	576	ARG	CZ-NH2	17.92	1.56	1.33
1	A	323	SER	CB-OG	-15.88	1.21	1.42
1	A	282	GLU	CD-OE2	15.06	1.42	1.25
1	B	326	GLU	CB-CG	-14.17	1.25	1.52
1	A	422	SER	CA-CB	13.91	1.73	1.52
1	B	282	GLU	CD-OE2	13.72	1.40	1.25
1	B	301	TYR	CG-CD2	-12.82	1.22	1.39
1	A	559	GLU	CB-CG	-11.42	1.30	1.52
1	B	224	MET	CB-CG	10.96	1.86	1.51
1	A	544	ARG	CD-NE	10.92	1.65	1.46
1	A	559	GLU	CG-CD	10.00	1.67	1.51
1	A	544	ARG	NE-CZ	-9.84	1.20	1.33
1	A	30	ASN	CG-OD1	-9.63	1.02	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	ALA	N-CA	9.55	1.65	1.46
1	A	282	GLU	CG-CD	9.13	1.65	1.51
1	A	348	GLU	CD-OE2	-9.05	1.15	1.25
1	A	642	SER	CB-OG	8.99	1.53	1.42
1	A	701	VAL	CB-CG1	-8.98	1.33	1.52
1	B	301	TYR	CE2-CZ	-8.80	1.27	1.38
1	B	446	GLN	CG-CD	8.77	1.71	1.51
1	B	642	SER	CA-CB	8.76	1.66	1.52
1	B	580	TYR	CZ-OH	-8.70	1.23	1.37
1	B	282	GLU	CG-CD	8.67	1.65	1.51
1	A	579	LYS	CD-CE	8.40	1.72	1.51
1	A	247	ASP	CG-OD2	8.37	1.44	1.25
1	A	146	GLU	CD-OE1	-8.33	1.16	1.25
1	A	326	GLU	CB-CG	-8.12	1.36	1.52
1	A	345	GLU	CG-CD	-8.02	1.40	1.51
1	B	364	LYS	CG-CD	-7.95	1.25	1.52
1	B	364	LYS	CE-NZ	-7.57	1.30	1.49
1	A	544	ARG	CZ-NH2	-7.55	1.23	1.33
1	A	463	ARG	CB-CG	-7.53	1.32	1.52
1	A	23	GLU	CD-OE2	7.47	1.33	1.25
1	A	597	GLU	CD-OE2	-7.46	1.17	1.25
1	A	568	ARG	CD-NE	-7.44	1.33	1.46
1	A	546	ARG	CZ-NH1	-7.43	1.23	1.33
1	B	384	SER	CB-OG	-7.41	1.32	1.42
1	A	323	SER	CA-CB	7.31	1.64	1.52
1	B	296	ASP	CB-CG	-7.28	1.36	1.51
1	A	576	ARG	CD-NE	-7.25	1.34	1.46
1	B	560	THR	CA-CB	7.24	1.72	1.53
1	A	124	LEU	CG-CD1	-7.24	1.25	1.51
1	B	297	GLU	CG-CD	7.19	1.62	1.51
1	B	544	ARG	NE-CZ	-7.08	1.23	1.33
1	A	422	SER	CB-OG	-7.04	1.33	1.42
1	A	247	ASP	CB-CG	7.03	1.66	1.51
1	B	544	ARG	CG-CD	7.02	1.69	1.51
1	A	609	THR	CB-CG2	-7.00	1.29	1.52
1	A	599	ARG	CZ-NH2	-6.97	1.24	1.33
1	B	339	TYR	CE2-CZ	-6.89	1.29	1.38
1	A	576	ARG	CZ-NH2	-6.80	1.24	1.33
1	A	609	THR	CB-OG1	6.72	1.56	1.43
1	B	599	ARG	NE-CZ	6.67	1.41	1.33
1	A	544	ARG	CG-CD	6.64	1.68	1.51
1	B	568	ARG	CD-NE	-6.63	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	544	ARG	CD-NE	-6.61	1.35	1.46
1	A	587	GLN	CD-OE1	6.59	1.38	1.24
1	B	348	GLU	CD-OE2	-6.32	1.18	1.25
1	B	204	LYS	CD-CE	6.23	1.66	1.51
1	A	597	GLU	CB-CG	-6.21	1.40	1.52
1	A	586	ALA	CA-C	6.14	1.69	1.52
1	A	250	GLU	CD-OE1	6.12	1.32	1.25
1	A	147	ILE	CA-CB	-6.06	1.41	1.54
1	B	692	ARG	CZ-NH2	-5.99	1.25	1.33
1	A	384	SER	CB-OG	-5.97	1.34	1.42
1	A	559	GLU	C-O	5.93	1.34	1.23
1	B	429	SER	CB-OG	-5.92	1.34	1.42
1	B	546	ARG	CZ-NH1	-5.86	1.25	1.33
1	A	339	TYR	CE2-CZ	-5.81	1.30	1.38
1	B	338	GLU	CD-OE1	-5.81	1.19	1.25
1	A	580	TYR	CE2-CZ	-5.80	1.31	1.38
1	B	559	GLU	CD-OE1	-5.76	1.19	1.25
1	B	580	TYR	CE1-CZ	-5.71	1.31	1.38
1	A	30	ASN	CB-CG	5.67	1.64	1.51
1	A	456	SER	C-O	-5.57	1.12	1.23
1	A	264	TYR	CD1-CE1	-5.53	1.31	1.39
1	B	301	TYR	CG-CD1	5.52	1.46	1.39
1	A	147	ILE	CB-CG2	5.49	1.69	1.52
1	A	128	GLY	N-CA	5.45	1.54	1.46
1	A	338	GLU	CD-OE1	-5.44	1.19	1.25
1	B	186	ARG	CZ-NH2	-5.44	1.25	1.33
1	B	707	ALA	CA-CB	5.42	1.63	1.52
1	A	333	TRP	C-O	5.41	1.33	1.23
1	A	351	ARG	CZ-NH2	5.41	1.40	1.33
1	A	32	ARG	NE-CZ	5.38	1.40	1.33
1	B	323	SER	CB-OG	-5.34	1.35	1.42
1	B	422	SER	CA-CB	5.33	1.60	1.52
1	A	501	ILE	CG1-CD1	-5.33	1.13	1.50
1	A	104	ARG	C-O	5.31	1.33	1.23
1	B	188	VAL	CA-CB	5.29	1.65	1.54
1	A	243	THR	CA-CB	5.21	1.67	1.53
1	A	289	VAL	C-N	-5.20	1.22	1.34
1	B	147	ILE	CB-CG2	5.18	1.69	1.52
1	B	370	ARG	CZ-NH1	5.14	1.39	1.33
1	A	568	ARG	CG-CD	5.13	1.64	1.51
1	A	582	GLY	N-CA	-5.12	1.38	1.46
1	A	363	GLY	CA-C	5.10	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	546	ARG	CG-CD	5.07	1.64	1.51
1	A	147	ILE	CB-CG1	-5.04	1.40	1.54
1	B	193	LYS	CB-CG	-5.02	1.39	1.52
1	A	143	ARG	CZ-NH1	-5.01	1.26	1.33

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	576	ARG	NE-CZ-NH2	26.03	133.31	120.30
1	B	576	ARG	NE-CZ-NH1	-24.48	108.06	120.30
1	B	370	ARG	NE-CZ-NH2	-24.04	108.28	120.30
1	B	370	ARG	NE-CZ-NH1	18.53	129.56	120.30
1	A	77	ARG	NE-CZ-NH1	14.62	127.61	120.30
1	B	224	MET	CG-SD-CE	-13.77	78.17	100.20
1	A	370	ARG	NE-CZ-NH1	12.77	126.69	120.30
1	A	692	ARG	NE-CZ-NH2	-12.57	114.01	120.30
1	A	701	VAL	CG1-CB-CG2	12.04	130.16	110.90
1	A	77	ARG	NE-CZ-NH2	-11.82	114.39	120.30
1	A	23	GLU	OE1-CD-OE2	11.75	137.40	123.30
1	A	455	ASP	CB-CG-OD2	11.58	128.72	118.30
1	A	576	ARG	NE-CZ-NH1	11.42	126.01	120.30
1	B	599	ARG	NE-CZ-NH1	10.95	125.78	120.30
1	A	247	ASP	CB-CG-OD2	10.78	128.00	118.30
1	B	690	GLU	OE1-CD-OE2	-10.58	110.60	123.30
1	A	32	ARG	NE-CZ-NH1	10.30	125.45	120.30
1	A	568	ARG	NE-CZ-NH2	-10.24	115.18	120.30
1	A	559	GLU	OE1-CD-OE2	-10.11	111.17	123.30
1	B	692	ARG	NE-CZ-NH1	10.05	125.32	120.30
1	A	242	ALA	CB-CA-C	-10.01	95.08	110.10
1	A	370	ARG	NE-CZ-NH2	-9.77	115.42	120.30
1	B	692	ARG	NE-CZ-NH2	-9.77	115.42	120.30
1	A	544	ARG	NE-CZ-NH2	9.73	125.17	120.30
1	B	401	GLU	OE1-CD-OE2	9.52	134.72	123.30
1	B	77	ARG	CD-NE-CZ	9.44	136.82	123.60
1	B	568	ARG	NE-CZ-NH1	9.33	124.96	120.30
1	A	599	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	A	124	LEU	CB-CG-CD2	8.90	126.13	111.00
1	B	699	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	A	455	ASP	CB-CG-OD1	-8.72	110.46	118.30
1	A	457	SER	C-N-CD	8.51	146.27	128.40
1	B	297	GLU	CG-CD-OE2	8.31	134.93	118.30
1	B	580	TYR	CB-CG-CD1	8.30	125.98	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	A	576	ARG	CG-CD-NE	-8.13	94.72	111.80
1	A	544	ARG	NE-CZ-NH1	-8.11	116.25	120.30
1	B	568	ARG	CG-CD-NE	-8.03	94.94	111.80
1	A	576	ARG	CD-NE-CZ	-8.02	112.37	123.60
1	A	463	ARG	CG-CD-NE	-8.00	94.99	111.80
1	A	242	ALA	N-CA-CB	7.82	121.05	110.10
1	B	297	GLU	CG-CD-OE1	-7.80	102.69	118.30
1	A	599	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	B	308	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	B	497	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	B	576	ARG	CD-NE-CZ	7.31	133.83	123.60
1	A	32	ARG	NH1-CZ-NH2	-7.28	111.39	119.40
1	B	351	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	B	290	ASP	CB-CG-OD2	7.13	124.72	118.30
1	B	308	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	B	329	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	B	699	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	690	GLU	CG-CD-OE1	6.70	131.70	118.30
1	B	113	ARG	NE-CZ-NH2	6.69	123.64	120.30
1	A	703	LYS	CD-CE-NZ	6.67	127.04	111.70
1	A	193	LYS	CD-CE-NZ	-6.65	96.41	111.70
1	A	564	ASP	CB-CG-OD1	6.61	124.25	118.30
1	A	592	TYR	CB-CG-CD2	6.58	124.95	121.00
1	B	373	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	364	LYS	CD-CE-NZ	-6.45	96.88	111.70
1	A	544	ARG	CG-CD-NE	6.39	125.22	111.80
1	A	633	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	B	386	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	A	293	LEU	CB-CG-CD1	6.17	121.48	111.00
1	B	364	LYS	CD-CE-NZ	-6.11	97.64	111.70
1	B	599	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	654	TYR	CB-CG-CD1	6.06	124.63	121.00
1	A	89	ASP	CB-CG-OD1	6.03	123.73	118.30
1	A	684	VAL	CA-CB-CG2	5.97	119.85	110.90
1	B	282	GLU	CG-CD-OE1	-5.90	106.50	118.30
1	B	401	GLU	CG-CD-OE2	-5.86	106.57	118.30
1	A	382	THR	CA-CB-CG2	-5.83	104.24	112.40
1	A	282	GLU	CG-CD-OE1	-5.79	106.73	118.30
1	A	186	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	329	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	282	GLU	CG-CD-OE2	5.76	129.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	544	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	560	THR	CA-CB-CG2	-5.68	104.45	112.40
1	A	384	SER	N-CA-CB	-5.66	102.01	110.50
1	B	119	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	23	GLU	CG-CD-OE2	-5.56	107.18	118.30
1	B	351	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	290	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	119	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	A	32	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	A	58	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	B	320	TYR	CB-CG-CD1	5.46	124.27	121.00
1	A	568	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	A	626	HIS	CG-ND1-CE1	-5.42	98.65	105.70
1	B	326	GLU	CB-CG-CD	5.42	128.83	114.20
1	A	573	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	351	ARG	NE-CZ-NH1	-5.39	117.61	120.30
1	A	703	LYS	CA-CB-CG	5.37	125.21	113.40
1	A	386	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	501	ILE	CB-CG1-CD1	5.33	128.82	113.90
1	B	384	SER	N-CA-CB	-5.32	102.52	110.50
1	B	51	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	301	TYR	CD1-CE1-CZ	-5.24	115.09	119.80
1	B	146	GLU	OE1-CD-OE2	-5.21	117.04	123.30
1	A	186	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	58	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	386	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	648	PHE	CB-CG-CD2	5.14	124.40	120.80
1	B	326	GLU	CA-CB-CG	5.11	124.63	113.40
1	A	290	ASP	C-N-CA	-5.09	111.61	122.30
1	A	457	SER	N-CA-C	5.09	124.74	111.00
1	B	405	PHE	CB-CG-CD1	5.06	124.34	120.80
1	A	457	SER	C-N-CA	-5.03	100.86	122.00
1	B	349	PHE	CB-CG-CD1	5.03	124.32	120.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	THR	Mainchain
1	A	291	GLY	Peptide
1	A	430	GLN	Sidechain
1	A	456	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	A	654	TYR	Sidechain
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	97	0
1	B	5212	0	5102	72	0
2	A	15	0	0	1	0
2	B	5	0	0	0	0
3	A	53	0	31	0	0
3	B	53	0	31	1	0
4	A	12	0	15	0	0
4	B	12	0	16	0	0
5	A	1100	0	0	70	4
5	B	1109	0	0	48	4
All	All	12783	0	10297	166	4

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 8.

All (166) 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:B:224:MET:CB	1:B:224:MET:CG	1.86	1.53
1:A:247:ASP:HB3	5:A:4094:HOH:O	1.22	1.37
1:B:579:LYS:HE3	5:B:2989:HOH:O	1.37	1.22
1:B:164:PRO:HG2	5:B:2996:HOH:O	1.33	1.21
1:B:707:ALA:HB2	5:B:2805:HOH:O	1.37	1.19
1:A:690:GLU:HG3	5:A:4085:HOH:O	1.00	1.16
1:A:699:ARG:NH1	5:A:3581:HOH:O	1.79	1.14
1:A:576:ARG:NH1	5:A:3697:HOH:O	1.67	1.13
1:B:576:ARG:NH1	5:B:2995:HOH:O	1.76	1.12
1:A:356:LYS:HE2	5:A:4033:HOH:O	1.52	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:ARG:NE	5:A:3668:HOH:O	1.87	1.07
1:A:243:THR:CG2	5:A:4028:HOH:O	2.01	1.06
1:A:291:GLY:HA2	5:A:3987:HOH:O	1.55	1.06
1:B:282:GLU:HG3	5:B:2335:HOH:O	1.55	1.06
1:B:166:LYS:NZ	5:B:2856:HOH:O	1.87	1.06
1:A:58:ARG:CZ	5:A:4076:HOH:O	2.02	1.05
1:A:707:ALA:HA	5:A:4032:HOH:O	1.55	1.05
1:B:290:ASP:OD2	1:B:292:VAL:HG12	1.60	1.01
1:A:707:ALA:HA	5:A:4074:HOH:O	1.60	0.97
5:A:3786:HOH:O	1:B:301:TYR:CE1	2.17	0.97
1:A:243:THR:HG22	5:A:4028:HOH:O	1.60	0.97
1:A:282:GLU:HG3	5:A:3474:HOH:O	1.69	0.93
1:B:526:ALA:N	5:B:2979:HOH:O	2.04	0.90
1:B:379:HIS:HE1	1:B:646:ARG:H	1.18	0.89
1:A:576:ARG:CZ	5:A:3668:HOH:O	2.17	0.89
1:A:707:ALA:CB	5:A:4074:HOH:O	2.20	0.89
1:A:413:ASP:HB3	5:A:4012:HOH:O	1.72	0.88
1:A:705:PRO:O	5:A:4092:HOH:O	1.91	0.86
1:B:290:ASP:OD2	1:B:292:VAL:CG1	2.24	0.85
1:B:292:VAL:HA	5:B:2980:HOH:O	1.76	0.84
1:A:254:THR:HG22	5:A:4039:HOH:O	1.79	0.83
1:A:707:ALA:HB1	5:A:3207:HOH:O	1.76	0.83
1:B:104:ARG:HA	5:B:2982:HOH:O	1.80	0.81
1:B:254:THR:HG22	5:B:2958:HOH:O	1.81	0.80
5:A:3936:HOH:O	1:B:293:LEU:HD23	1.81	0.80
1:A:576:ARG:NH2	5:A:3668:HOH:O	2.14	0.80
1:A:289:VAL:O	1:A:290:ASP:OD2	1.99	0.79
1:A:51:ARG:NH1	5:A:4100:HOH:O	2.16	0.79
1:A:204:LYS:HB2	1:A:204:LYS:NZ	1.98	0.78
1:A:559:GLU:O	5:A:4052:HOH:O	2.02	0.77
1:A:626:HIS:CD2	5:B:2305:HOH:O	2.39	0.76
1:B:703:LYS:NZ	5:B:2766:HOH:O	2.15	0.75
1:A:51:ARG:NH1	5:A:4056:HOH:O	2.10	0.75
1:A:706:ALA:O	1:A:707:ALA:HB2	1.86	0.75
1:A:540:ASP:OD2	1:B:472:HIS:HD2	1.71	0.73
1:B:218:GLN:NE2	5:B:2765:HOH:O	2.00	0.73
1:A:472:HIS:HE1	1:A:539:GLU:OE2	1.71	0.73
1:B:104:ARG:CA	5:B:2982:HOH:O	2.37	0.72
1:A:472:HIS:HD2	1:B:540:ASP:OD2	1.72	0.72
1:A:243:THR:HG21	5:A:4028:HOH:O	1.78	0.71
1:B:193:LYS:NZ	5:B:2877:HOH:O	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LYS:HB2	1:A:204:LYS:HZ2	1.55	0.71
1:A:644:ASP:OD1	5:A:3637:HOH:O	2.09	0.70
1:A:626:HIS:HE1	5:A:3228:HOH:O	1.75	0.70
1:A:422:SER:HB3	5:A:3365:HOH:O	1.91	0.70
1:B:472:HIS:HE1	1:B:539:GLU:OE2	1.74	0.69
1:B:77:ARG:HD3	5:B:2077:HOH:O	1.92	0.69
1:A:455:ASP:OD1	5:A:4101:HOH:O	2.12	0.68
1:A:16:LYS:CA	5:A:4090:HOH:O	2.40	0.68
1:A:16:LYS:N	5:A:4098:HOH:O	2.27	0.68
1:A:58:ARG:NH1	5:A:4076:HOH:O	2.15	0.68
1:A:413:ASP:CB	5:A:4012:HOH:O	2.35	0.66
1:B:224:MET:SD	1:B:224:MET:CB	2.82	0.66
1:A:16:LYS:HA	5:A:4090:HOH:O	1.96	0.65
1:A:193:LYS:N	1:A:193:LYS:HD3	2.08	0.65
5:A:3786:HOH:O	1:B:301:TYR:HE1	1.67	0.64
1:A:124:LEU:HD13	1:A:124:LEU:C	2.18	0.64
1:A:587:GLN:NE2	5:A:3922:HOH:O	2.06	0.64
1:B:412:HIS:HD2	1:B:653:SER:OG	1.81	0.64
1:A:30:ASN:OD1	5:A:4072:HOH:O	2.15	0.64
5:A:3786:HOH:O	1:B:301:TYR:CD1	2.47	0.64
1:B:393:ASP:OD2	1:B:399:HIS:HE1	1.79	0.63
1:A:412:HIS:HD2	1:A:653:SER:OG	1.82	0.63
1:B:102:HIS:HD2	5:B:2237:HOH:O	1.80	0.63
1:B:153:HIS:HE1	5:B:1986:HOH:O	1.81	0.63
1:B:707:ALA:C	5:B:3005:HOH:O	2.36	0.62
1:A:51:ARG:NH2	5:A:4056:HOH:O	2.28	0.62
1:A:639:LEU:O	1:A:707:ALA:CB	2.47	0.62
1:B:446:GLN:OE1	5:B:2998:HOH:O	2.16	0.62
1:A:639:LEU:O	1:A:707:ALA:HB3	2.00	0.62
1:A:544:ARG:NH1	5:A:3300:HOH:O	2.32	0.61
1:B:289:VAL:HB	1:B:293:LEU:HD12	1.81	0.61
1:B:379:HIS:CE1	1:B:646:ARG:H	2.10	0.61
1:A:16:LYS:HB3	5:A:4090:HOH:O	2.01	0.61
1:A:559:GLU:CD	5:A:3334:HOH:O	2.39	0.60
1:B:707:ALA:CB	5:B:2805:HOH:O	2.16	0.60
1:A:705:PRO:HG3	5:A:3281:HOH:O	2.01	0.60
1:A:393:ASP:OD2	1:A:399:HIS:HE1	1.84	0.59
1:A:706:ALA:O	1:A:707:ALA:CB	2.50	0.59
1:A:193:LYS:HD2	5:A:3483:HOH:O	2.03	0.59
1:B:699:ARG:NH2	5:B:2890:HOH:O	2.35	0.59
1:B:250:GLU:OE2	1:B:254:THR:HG21	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ASP:CB	5:A:4094:HOH:O	2.04	0.59
1:B:164:PRO:HB3	5:B:3000:HOH:O	2.01	0.58
1:B:696:ILE:HD11	5:B:2447:HOH:O	2.01	0.58
1:A:626:HIS:CE1	5:A:3228:HOH:O	2.53	0.57
1:B:263:GLN:HG3	5:B:2988:HOH:O	2.04	0.57
1:A:544:ARG:HD2	5:A:3283:HOH:O	2.03	0.57
1:B:351:ARG:CD	5:B:2910:HOH:O	2.53	0.56
1:B:703:LYS:HD2	5:B:2766:HOH:O	2.04	0.56
1:A:547:HIS:HE1	5:A:4003:HOH:O	1.87	0.56
1:A:626:HIS:HD2	1:B:296:ASP:OD1	1.89	0.56
1:B:104:ARG:HD2	5:B:2713:HOH:O	2.06	0.56
1:A:23:GLU:OE1	5:A:3452:HOH:O	2.18	0.56
1:A:457:SER:O	1:A:458:PRO:C	2.42	0.56
1:A:58:ARG:NE	5:A:4076:HOH:O	2.25	0.55
1:B:224:MET:CB	1:B:224:MET:CE	2.85	0.55
1:B:164:PRO:CG	5:B:2996:HOH:O	2.12	0.55
1:A:707:ALA:HB1	5:A:4074:HOH:O	1.98	0.54
1:B:292:VAL:CG2	5:B:2954:HOH:O	2.56	0.54
1:B:351:ARG:HD2	5:B:2910:HOH:O	2.08	0.54
1:A:193:LYS:CD	5:A:3483:HOH:O	2.57	0.53
1:A:361:GLY:C	5:A:4010:HOH:O	2.48	0.52
5:A:3768:HOH:O	1:B:301:TYR:CE1	2.54	0.52
1:A:243:THR:CG2	5:A:3245:HOH:O	2.58	0.52
1:A:707:ALA:CA	5:A:4074:HOH:O	2.26	0.52
1:B:282:GLU:CG	5:B:2335:HOH:O	2.32	0.52
1:A:559:GLU:CD	5:A:4084:HOH:O	2.49	0.51
1:A:143:ARG:HH11	1:A:170:ASN:ND2	2.08	0.51
1:A:245:PRO:HA	5:A:3544:HOH:O	2.11	0.50
1:B:224:MET:HB2	1:B:224:MET:CE	2.42	0.50
1:A:242:ALA:HB1	5:A:3767:HOH:O	2.11	0.50
1:A:289:VAL:O	1:A:290:ASP:CG	2.50	0.49
1:B:94:GLU:O	1:B:102:HIS:HE1	1.95	0.49
1:A:546:ARG:NE	2:A:3001:SO4:O4	2.42	0.49
1:B:290:ASP:OD1	1:B:290:ASP:C	2.51	0.49
1:A:243:THR:HG21	5:A:3245:HOH:O	2.14	0.48
1:B:282:GLU:HG2	5:B:2685:HOH:O	2.12	0.48
1:B:33:HIS:CE1	1:B:657:LEU:HD11	2.49	0.48
1:A:33:HIS:CE1	1:A:657:LEU:HD11	2.49	0.47
1:B:104:ARG:C	5:B:2982:HOH:O	2.51	0.47
5:A:3768:HOH:O	1:B:301:TYR:CD1	2.66	0.47
1:A:78:LEU:HD11	1:A:676:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ARG:HD3	5:B:2910:HOH:O	2.14	0.46
1:A:587:GLN:NE2	1:A:587:GLN:HA	2.31	0.46
1:A:166:LYS:CE	5:A:4082:HOH:O	2.63	0.46
1:A:413:ASP:HB3	5:B:2329:HOH:O	2.14	0.46
1:B:141:ALA:HA	3:B:801:FAD:C4X	2.46	0.46
1:B:446:GLN:HG2	5:B:2998:HOH:O	2.16	0.46
1:B:224:MET:HE3	5:B:2762:HOH:O	2.15	0.46
1:B:692:ARG:NH1	5:B:2885:HOH:O	2.48	0.45
1:B:584:SER:HA	5:B:2893:HOH:O	2.16	0.45
1:A:166:LYS:HE3	5:A:4082:HOH:O	2.15	0.45
1:B:164:PRO:HD3	5:B:3000:HOH:O	2.16	0.45
1:A:245:PRO:CA	5:A:3544:HOH:O	2.65	0.44
1:B:292:VAL:HG23	5:B:2954:HOH:O	2.16	0.44
1:A:204:LYS:CB	1:A:204:LYS:NZ	2.70	0.44
1:A:408:LEU:HD13	1:A:415:LEU:HD11	1.99	0.43
1:A:579:LYS:HE3	1:A:583:ALA:O	2.18	0.43
1:A:204:LYS:HB2	1:A:204:LYS:HZ3	1.79	0.43
1:A:340:THR:HG21	5:A:3608:HOH:O	2.18	0.43
1:A:576:ARG:NH1	1:A:576:ARG:CG	2.81	0.42
1:B:359:ASN:ND2	5:B:2720:HOH:O	2.52	0.42
1:A:51:ARG:CZ	5:A:4056:HOH:O	2.52	0.42
1:A:559:GLU:C	5:A:4052:HOH:O	2.56	0.42
1:B:579:LYS:CD	5:B:2989:HOH:O	2.63	0.42
1:A:626:HIS:HD2	5:B:2305:HOH:O	1.86	0.41
1:B:292:VAL:HG22	5:B:2954:HOH:O	2.18	0.41
1:A:587:GLN:HE21	1:A:587:GLN:HA	1.85	0.41
1:A:417:PRO:HB2	5:A:3311:HOH:O	2.21	0.41
1:B:39:VAL:HB	1:B:693:PRO:HB2	2.03	0.41
1:A:143:ARG:HH11	1:A:170:ASN:HD21	1.67	0.41
1:A:399:HIS:HD2	5:A:3566:HOH:O	2.03	0.41
1:B:455:ASP:OD2	5:B:2438:HOH:O	2.21	0.41
1:B:193:LYS:HG2	1:B:193:LYS:O	2.21	0.41
1:A:586:ALA:HB2	5:B:2110:HOH:O	2.21	0.40

All (4) 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)
5:A:3444:HOH:O	5:B:2669:HOH:O[4_556]	1.83	0.37
5:A:3981:HOH:O	5:B:2824:HOH:O[2_664]	1.98	0.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:3241:HOH:O	5:B:2104:HOH:O[4_556]	2.03	0.17
5:A:3372:HOH:O	5:B:2461:HOH:O[3_756]	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%)	16 (2%)	1 (0%)	51	19
1	B	678/721 (94%)	665 (98%)	13 (2%)	0	100	100
All	All	1356/1442 (94%)	1326 (98%)	29 (2%)	1 (0%)	51	19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	457	SER

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	534/566 (94%)	532 (100%)	2 (0%)	91	77
1	B	534/566 (94%)	533 (100%)	1 (0%)	93	80
All	All	1068/1132 (94%)	1065 (100%)	3 (0%)	92	79

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	ASP
1	A	701	VAL
1	B	326	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	170	ASN
1	A	216	ASN
1	A	399	HIS
1	A	412	HIS
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	396	ASN
1	B	399	HIS
1	B	412	HIS
1	B	446	GLN
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](#)

10 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	1903	-	4,4,4	0.46	0	6,6,6	0.45	0
4	GOL	B	1901	-	5,5,5	0.81	0	5,5,5	0.92	0
2	SO4	A	3001	-	4,4,4	1.42	0	6,6,6	5.00	6 (100%)
2	SO4	A	903	-	4,4,4	0.26	0	6,6,6	0.45	0
4	GOL	A	902	-	5,5,5	1.03	0	5,5,5	0.72	0
4	GOL	B	1902	-	5,5,5	0.66	0	5,5,5	0.69	0
3	FAD	B	801	-	51,58,58	1.53	7 (13%)	60,89,89	1.64	6 (10%)
2	SO4	A	3002	-	4,4,4	1.78	2 (50%)	6,6,6	3.20	2 (33%)
4	GOL	A	901	-	5,5,5	0.30	0	5,5,5	0.79	0
3	FAD	A	801	-	51,58,58	1.53	10 (19%)	60,89,89	1.71	5 (8%)

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
4	GOL	B	1901	-	-	0/4/4/4	-
4	GOL	A	902	-	-	0/4/4/4	-
4	GOL	B	1902	-	-	0/4/4/4	-
3	FAD	B	801	-	-	3/30/50/50	0/6/6/6
4	GOL	A	901	-	-	0/4/4/4	-
3	FAD	A	801	-	-	3/30/50/50	0/6/6/6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	FAD	C4X-N5	4.51	1.39	1.33
3	A	801	FAD	C4X-N5	4.28	1.39	1.33
3	B	801	FAD	C4-N3	3.95	1.39	1.33
3	B	801	FAD	O4B-C1B	3.69	1.46	1.41
3	A	801	FAD	C2'-C3'	3.65	1.60	1.53
3	B	801	FAD	C9A-N10	3.03	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	FAD	C6-C5X	-2.91	1.37	1.41
3	A	801	FAD	C5'-C4'	2.83	1.55	1.51
3	A	801	FAD	C10-N1	2.69	1.36	1.33
3	A	801	FAD	C2B-C1B	-2.68	1.49	1.53
3	B	801	FAD	C5X-N5	2.62	1.39	1.35
2	A	3002	SO4	O2-S	-2.56	1.32	1.46
3	A	801	FAD	C4-N3	2.49	1.37	1.33
3	A	801	FAD	O4B-C1B	2.48	1.44	1.41
3	B	801	FAD	C1'-N10	-2.21	1.46	1.48
3	A	801	FAD	C9-C9A	-2.21	1.36	1.40
3	A	801	FAD	C6-C5X	-2.16	1.38	1.41
3	A	801	FAD	C4'-C3'	-2.16	1.49	1.53
2	A	3002	SO4	O4-S	2.03	1.64	1.47

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	FAD	C4-N3-C2	8.89	122.65	115.14
2	A	3001	SO4	O3-S-O1	-8.25	66.26	109.31
3	B	801	FAD	C4-N3-C2	6.62	120.73	115.14
2	A	3002	SO4	O3-S-O2	-6.00	78.00	109.31
2	A	3001	SO4	O4-S-O2	5.19	136.41	109.31
3	A	801	FAD	C4X-C4-N3	-4.89	116.74	123.43
2	A	3001	SO4	O4-S-O3	4.69	129.06	109.06
2	A	3002	SO4	O2-S-O1	4.46	142.38	109.43
2	A	3001	SO4	O4-S-O1	-4.31	86.80	109.31
3	B	801	FAD	C4X-C4-N3	-4.29	117.56	123.43
3	B	801	FAD	C5'-C4'-C3'	-4.12	104.24	112.20
3	A	801	FAD	C5'-C4'-C3'	-3.83	104.81	112.20
3	A	801	FAD	C1'-N10-C9A	3.61	121.13	118.29
3	B	801	FAD	C1'-N10-C9A	3.55	121.09	118.29
2	A	3001	SO4	O3-S-O2	-3.12	93.02	109.31
3	B	801	FAD	C5A-C6A-N6A	2.60	124.30	120.35
2	A	3001	SO4	O2-S-O1	2.23	125.88	109.43
3	A	801	FAD	C3B-C2B-C1B	2.21	104.31	100.98
3	B	801	FAD	O4B-C1B-C2B	-2.17	103.76	106.93

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	801	FAD	PA-O3P-P-O5'

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

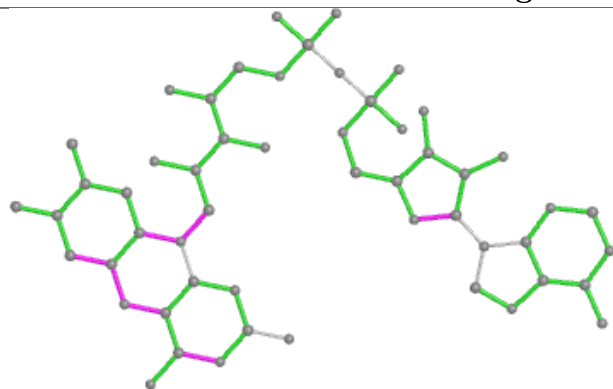
There are no ring outliers.

2 monomers are involved in 2 short contacts:

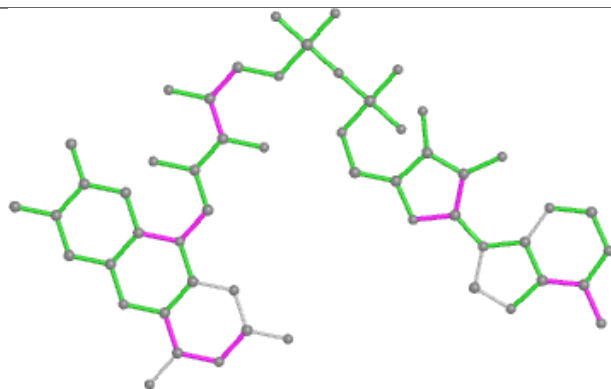
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3001	SO4	1	0
3	B	801	FAD	1	0

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.

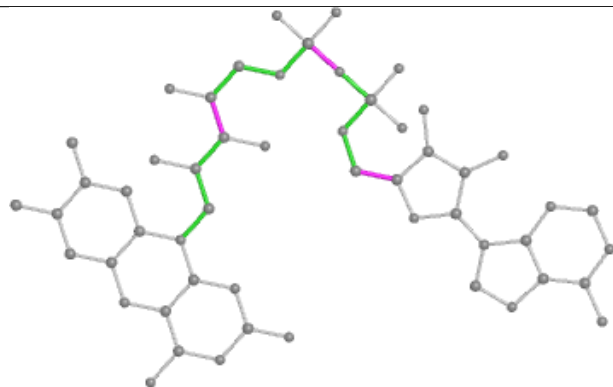
Ligand FAD B 801



Bond lengths



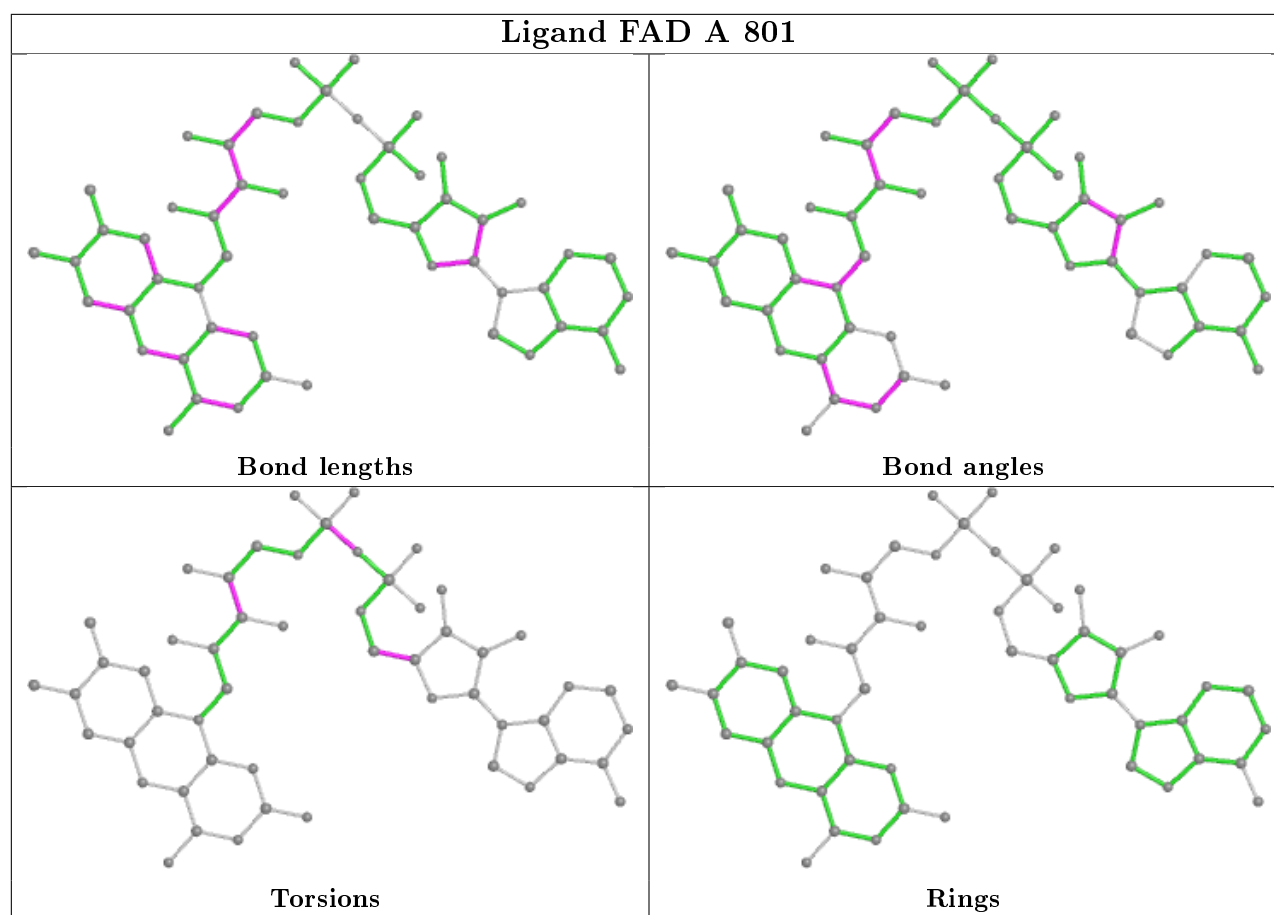
Bond angles



Torsions



Rings



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%)	-0.35	22 (3%)	47 39	6, 11, 25, 44	0
1	B	684/721 (94%)	-0.37	24 (3%)	44 36	6, 11, 26, 41	0
All	All	1368/1442 (94%)	-0.36	46 (3%)	45 37	6, 11, 25, 44	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	362	ALA	8.7
1	A	521	VAL	8.5
1	B	707	ALA	8.2
1	B	521	VAL	7.4
1	A	707	ALA	6.7
1	B	293	LEU	6.3
1	B	585	ASN	6.1
1	A	104	ARG	5.9
1	A	131	ALA	5.0
1	A	292	VAL	5.0
1	A	132	SER	4.7
1	A	130	PRO	4.7
1	B	292	VAL	4.6
1	B	583	ALA	4.6
1	A	128	GLY	4.4
1	A	496	TRP	4.3
1	A	16	LYS	4.3
1	B	581	ALA	4.0
1	B	526	ALA	3.6
1	A	291	GLY	3.6
1	B	246	ALA	3.4
1	B	584	SER	3.4
1	B	16	LYS	3.4
1	A	498	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	104	ARG	3.2
1	B	582	GLY	3.1
1	A	706	ALA	2.9
1	B	17	ILE	2.9
1	A	584	SER	2.9
1	B	586	ALA	2.9
1	A	497	ARG	2.7
1	A	127	ASN	2.6
1	B	130	PRO	2.5
1	B	580	TYR	2.4
1	B	706	ALA	2.3
1	A	129	ASP	2.3
1	B	132	SER	2.3
1	B	131	ALA	2.3
1	B	128	GLY	2.3
1	B	218	GLN	2.2
1	A	457	SER	2.2
1	A	526	ALA	2.1
1	A	85	GLY	2.1
1	B	127	ASN	2.1
1	B	129	ASP	2.0
1	A	705	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
4	GOL	A	901	6/6	0.96	0.07	11,13,14,15	0

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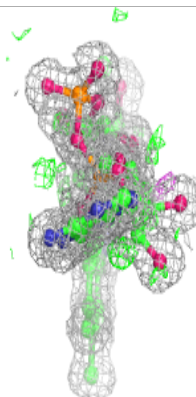
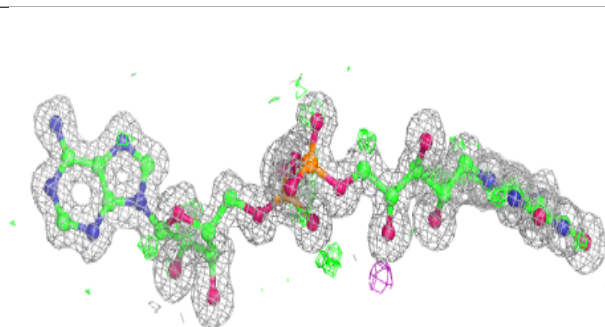
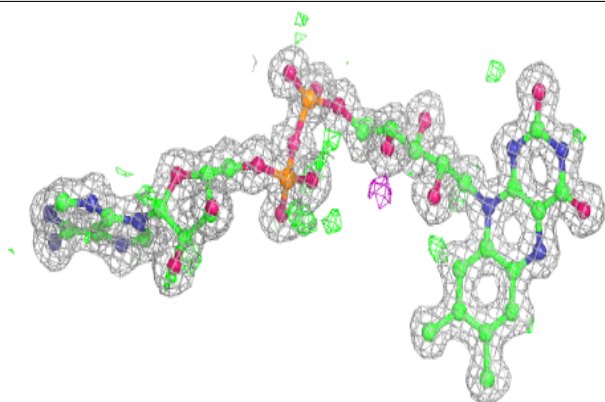
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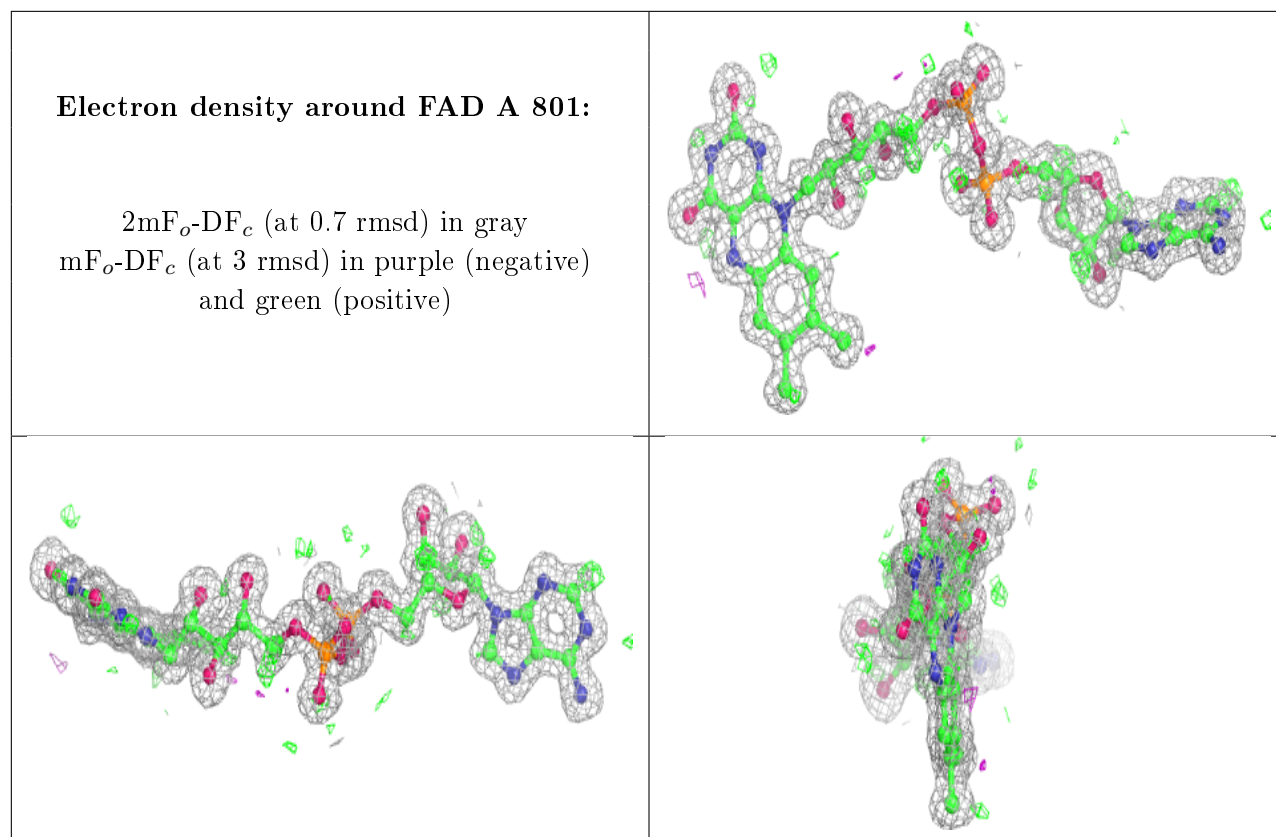
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	902	6/6	0.97	0.06	13,13,18,24	0
2	SO4	A	903	5/5	0.98	0.11	12,14,15,15	0
4	GOL	B	1901	6/6	0.98	0.06	10,12,13,13	0
4	GOL	B	1902	6/6	0.98	0.05	11,13,17,20	0
2	SO4	A	3001	5/5	0.98	0.06	17,18,29,30	0
3	FAD	B	801	53/53	0.99	0.06	6,6,7,8	0
2	SO4	A	3002	5/5	0.99	0.15	22,22,28,34	0
2	SO4	B	1903	5/5	0.99	0.05	12,13,13,14	0
3	FAD	A	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.