



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:47 AM UTC

PDB ID : 2YR6 / pdb_00002yr6
Title : Crystal structure of L-phenylalanine oxidase from Psuedomonas sp.P501
Authors : Ida, K.; Kurabayashi, M.; Suguro, M.; Suzuki, H.
Deposited on : 2007-04-02
Resolution : 1.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

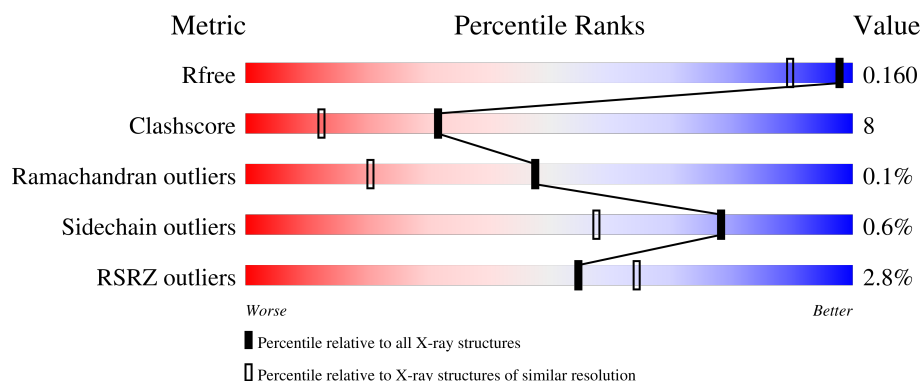
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

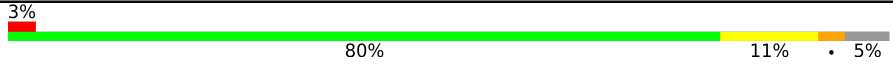
The reported resolution of this entry is 1.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1216 (1.36-1.36)
Clashscore	190562	1232 (1.36-1.36)
Ramachandran outliers	187476	1220 (1.36-1.36)
Sidechain outliers	187428	1220 (1.36-1.36)
RSRZ outliers	180081	1214 (1.36-1.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	721	
1	B	721	

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	3002	-	X	-	-
2	SO4	B	3001	-	X	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12529 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.

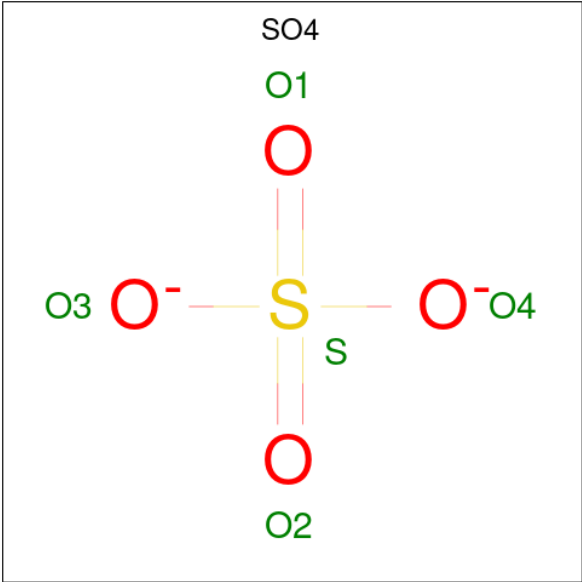
- Molecule 1 is a protein called Pro-enzyme of L-phenylalanine oxidase.

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:

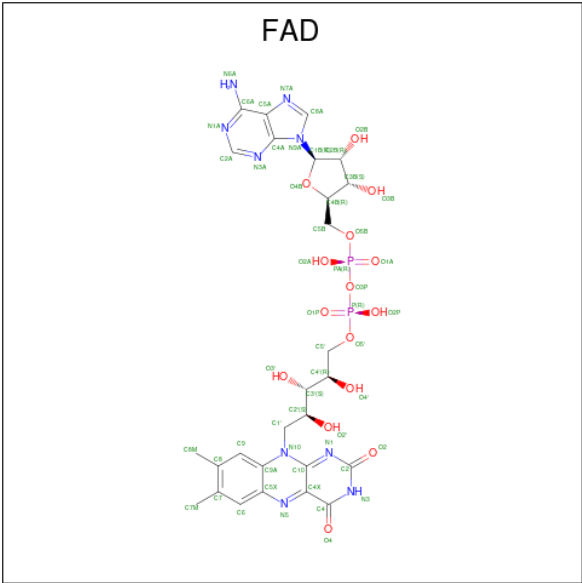
Chain	Residue	Modelled	Actual	Comment	Reference
A	714	LEU	-	expression tag	UNP Q5W9R9
A	715	GLU	-	expression tag	UNP Q5W9R9
A	716	HIS	-	expression tag	UNP Q5W9R9
A	717	HIS	-	expression tag	UNP Q5W9R9
A	718	HIS	-	expression tag	UNP Q5W9R9
A	719	HIS	-	expression tag	UNP Q5W9R9
A	720	HIS	-	expression tag	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 (CCD ID: SO4) (formula: O₄S).



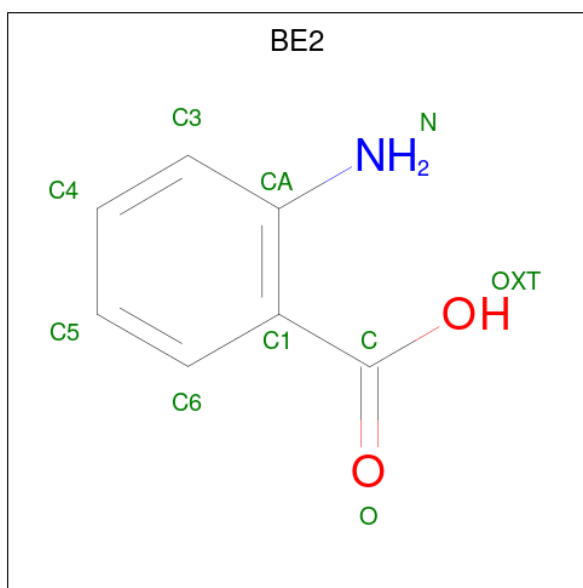
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



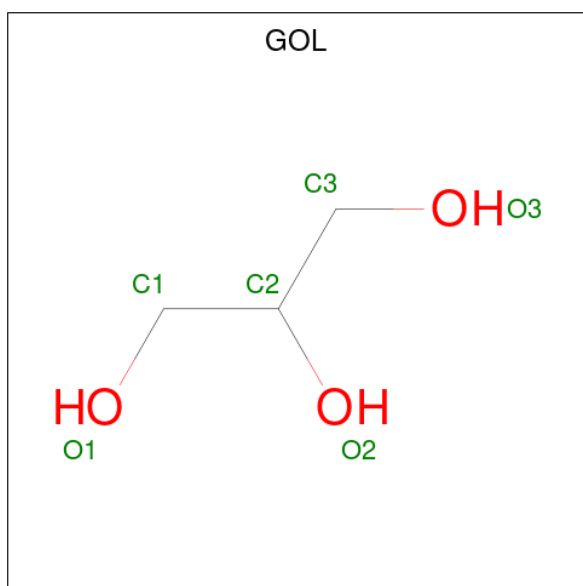
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0
			53	27	9	15	2	
3	B	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 4 is 2-AMINO BENZOIC ACID (CCD ID: BE2) (formula: $C_7H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	7	1	2		
4	B	1	Total	C	N	O	0	0
			10	7	1	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1000	Total	O	0	0
			1000	1000		
6	B	957	Total	O	0	0
			957	957		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.88Å 113.03Å 136.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.18 – 1.35 34.18 – 1.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.18-1.35) 99.8 (34.18-1.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.103 , 0.138 (Not available) , 0.160	Depositor DCC
R_{free} test set	17132 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	11.7	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	12529	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: SO4, FAD, BE2, GOL

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	1.80	83/5347 (1.6%)	1.51	61/7300 (0.8%)
1	B	1.69	62/5347 (1.2%)	1.41	46/7300 (0.6%)
All	All	1.75	145/10694 (1.4%)	1.46	107/14600 (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	7
1	B	0	6
All	All	0	13

All (145) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246	ALA	C-O	23.62	1.51	1.24
1	A	245	PRO	N-CA	22.39	1.75	1.47
1	A	576	ARG	CZ-NH1	16.49	1.55	1.32
1	B	224	MET	CB-CG	14.36	1.95	1.52
1	B	576	ARG	CZ-NH2	13.56	1.51	1.33
1	A	147	ILE	CB-CG1	-13.31	1.26	1.53
1	B	297	GLU	CD-OE2	12.60	1.49	1.25
1	B	544	ARG	CD-NE	12.55	1.63	1.46
1	A	245	PRO	C-O	12.11	1.39	1.24
1	A	576	ARG	CD-NE	-12.09	1.29	1.46
1	A	245	PRO	CA-C	11.99	1.69	1.52
1	B	292	VAL	N-CA	11.62	1.60	1.46
1	A	544	ARG	NE-CZ	-11.45	1.20	1.33
1	A	544	ARG	CD-NE	11.03	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	576	ARG	NE-CZ	10.86	1.45	1.33
1	B	58	ARG	CZ-NH2	10.83	1.47	1.33
1	A	246	ALA	CA-CB	-10.76	1.36	1.53
1	A	323	SER	CA-CB	10.74	1.71	1.53
1	A	245	PRO	CB-CG	10.51	2.02	1.49
1	B	643	LEU	C-N	-9.95	1.22	1.33
1	A	246	ALA	C-N	9.86	1.47	1.34
1	A	244	PRO	C-O	-9.67	1.13	1.24
1	A	323	SER	CB-OG	-9.38	1.23	1.42
1	A	702	VAL	C-O	-9.35	1.14	1.24
1	A	77	ARG	CZ-NH2	-9.14	1.21	1.33
1	A	706	ALA	CA-CB	8.98	1.67	1.53
1	B	546	ARG	CZ-NH2	-8.92	1.21	1.33
1	B	544	ARG	CZ-NH2	-8.82	1.22	1.33
1	A	702	VAL	CA-C	8.76	1.63	1.52
1	B	568	ARG	CD-NE	-8.72	1.34	1.46
1	B	544	ARG	NE-CZ	-8.52	1.23	1.33
1	A	422	SER	CA-CB	8.43	1.66	1.53
1	A	147	ILE	CA-CB	-8.23	1.43	1.54
1	A	626	HIS	CG-ND1	8.02	1.47	1.38
1	A	243	THR	CA-CB	7.78	1.64	1.53
1	A	362	ALA	CA-CB	7.76	1.66	1.53
1	A	544	ARG	CZ-NH2	-7.74	1.23	1.33
1	A	147	ILE	CB-CG2	7.63	1.77	1.52
1	B	147	ILE	CB-CG1	-7.58	1.38	1.53
1	A	599	ARG	NE-CZ	7.55	1.41	1.33
1	A	642	SER	CB-OG	7.53	1.57	1.42
1	B	692	ARG	CZ-NH2	-7.52	1.23	1.33
1	A	576	ARG	CZ-NH2	-7.46	1.23	1.33
1	B	203	LEU	CB-CG	-7.36	1.38	1.53
1	B	370	ARG	CZ-NH2	-7.26	1.24	1.33
1	B	147	ILE	CA-CB	-7.22	1.44	1.54
1	B	296	ASP	CB-CG	-7.11	1.34	1.52
1	B	386	ARG	CB-CG	-7.07	1.31	1.52
1	B	642	SER	CA-CB	6.96	1.65	1.53
1	B	546	ARG	CZ-NH1	-6.95	1.23	1.32
1	A	626	HIS	ND1-CE1	6.91	1.39	1.32
1	A	568	ARG	NE-CZ	6.88	1.40	1.33
1	A	428	ALA	CA-CB	6.87	1.64	1.53
1	B	147	ILE	CB-CG2	6.84	1.75	1.52
1	A	568	ARG	CD-NE	-6.83	1.36	1.46
1	A	77	ARG	CD-NE	-6.76	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	587	GLN	CA-CB	-6.75	1.45	1.53
1	A	692	ARG	CZ-NH2	-6.74	1.24	1.33
1	B	609	THR	CA-CB	6.72	1.63	1.53
1	A	449	PRO	CA-CB	-6.68	1.47	1.53
1	A	241	ALA	CA-C	6.65	1.61	1.52
1	B	364	LYS	CE-NZ	-6.59	1.29	1.49
1	B	364	LYS	CG-CD	-6.54	1.32	1.52
1	B	188	VAL	CA-CB	6.50	1.64	1.54
1	B	77	ARG	CD-NE	-6.50	1.37	1.46
1	B	292	VAL	C-O	6.48	1.31	1.24
1	A	502	LYS	CG-CD	6.47	1.71	1.52
1	A	568	ARG	CG-CD	-6.47	1.33	1.52
1	A	516	VAL	N-CA	6.36	1.53	1.46
1	A	463	ARG	CB-CG	-6.33	1.33	1.52
1	B	210	ALA	CA-C	-6.28	1.44	1.52
1	A	626	HIS	CG-CD2	6.25	1.42	1.35
1	B	585	ASN	CA-C	-6.15	1.45	1.52
1	B	642	SER	CB-OG	6.15	1.54	1.42
1	B	609	THR	CB-CG2	-6.10	1.32	1.52
1	B	28	GLY	C-O	6.08	1.28	1.24
1	B	92	ILE	CB-CG1	-6.02	1.41	1.53
1	B	323	SER	CB-OG	-6.02	1.30	1.42
1	A	587	GLN	CD-OE1	5.99	1.34	1.23
1	B	293	LEU	N-CA	5.95	1.53	1.46
1	A	496	TRP	C-O	-5.93	1.17	1.24
1	B	58	ARG	CZ-NH1	5.92	1.41	1.32
1	B	77	ARG	NE-CZ	5.91	1.39	1.33
1	A	546	ARG	CG-CD	5.89	1.70	1.52
1	A	287	PRO	CA-C	-5.89	1.46	1.52
1	B	544	ARG	CG-CD	5.88	1.70	1.52
1	A	385	ALA	C-O	5.88	1.31	1.24
1	A	581	ALA	CA-C	-5.87	1.45	1.52
1	B	289	VAL	C-O	5.83	1.31	1.24
1	A	218	GLN	CD-OE1	5.81	1.34	1.23
1	A	455	ASP	CA-CB	5.78	1.63	1.53
1	A	293	LEU	CG-CD1	-5.75	1.33	1.52
1	A	383	ALA	CA-CB	-5.75	1.44	1.53
1	B	283	LYS	CB-CG	-5.75	1.35	1.52
1	A	128	GLY	N-CA	5.67	1.53	1.45
1	B	587	GLN	CA-C	-5.61	1.46	1.52
1	A	373	ARG	NE-CZ	-5.60	1.26	1.33
1	A	412	HIS	ND1-CE1	5.60	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	290	ASP	CB-CG	5.59	1.66	1.52
1	A	586	ALA	CA-C	5.56	1.60	1.52
1	A	699	ARG	CD-NE	-5.53	1.38	1.46
1	A	645	ASN	N-CA	5.50	1.52	1.46
1	A	204	LYS	CB-CG	-5.49	1.35	1.52
1	A	247	ASP	N-CA	-5.45	1.39	1.46
1	A	588	PRO	N-CD	5.45	1.55	1.47
1	A	368	GLN	C-O	-5.45	1.17	1.23
1	B	560	THR	CA-CB	5.44	1.63	1.53
1	B	40	SER	CA-CB	-5.39	1.46	1.53
1	B	425	GLU	C-O	-5.36	1.18	1.23
1	A	174	VAL	CA-C	5.35	1.57	1.52
1	B	609	THR	CB-OG1	5.34	1.52	1.43
1	B	32	ARG	CG-CD	-5.33	1.36	1.52
1	A	520	ILE	CA-C	5.31	1.57	1.53
1	A	584	SER	N-CA	-5.30	1.39	1.46
1	A	599	ARG	CZ-NH2	-5.30	1.26	1.33
1	B	204	LYS	CD-CE	5.29	1.68	1.52
1	A	520	ILE	C-N	-5.25	1.26	1.33
1	A	83	PRO	CA-C	-5.23	1.47	1.52
1	A	290	ASP	CG-OD2	5.23	1.35	1.25
1	B	518	SER	CA-C	-5.21	1.47	1.53
1	A	292	VAL	CA-CB	-5.20	1.47	1.54
1	B	203	LEU	CG-CD2	5.20	1.69	1.52
1	B	599	ARG	NE-CZ	5.20	1.38	1.33
1	A	684	VAL	CB-CG2	-5.20	1.35	1.52
1	B	204	LYS	CE-NZ	-5.18	1.33	1.49
1	A	265	ASP	CA-CB	-5.18	1.44	1.53
1	B	297	GLU	N-CA	-5.18	1.40	1.46
1	A	609	THR	CB-OG1	5.17	1.52	1.43
1	B	127	ASN	N-CA	5.17	1.52	1.46
1	B	252	ILE	CA-CB	-5.17	1.48	1.54
1	A	290	ASP	N-CA	5.16	1.53	1.46
1	B	297	GLU	CG-CD	5.16	1.65	1.52
1	B	224	MET	CA-C	-5.15	1.45	1.52
1	A	627	GLN	CG-CD	-5.10	1.39	1.52
1	A	265	ASP	CG-OD2	-5.09	1.15	1.25
1	B	516	VAL	CA-C	-5.08	1.48	1.53
1	B	263	GLN	CD-OE1	5.08	1.33	1.23
1	A	456	SER	CB-OG	5.07	1.52	1.42
1	A	77	ARG	CZ-NH1	5.07	1.39	1.32
1	B	21	VAL	CA-C	-5.06	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	422	SER	CA-CB	5.05	1.61	1.53
1	B	640	ALA	N-CA	5.04	1.52	1.46
1	A	127	ASN	CA-C	-5.03	1.46	1.52
1	A	579	LYS	CD-CE	5.02	1.67	1.52
1	B	383	ALA	N-CA	5.01	1.52	1.45

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	PRO	CA-C-N	-21.11	93.45	119.84
1	A	244	PRO	C-N-CA	-21.11	93.45	119.84
1	A	576	ARG	NE-CZ-NH1	14.05	135.55	121.50
1	B	576	ARG	NE-CZ-NH2	13.69	131.52	119.20
1	B	576	ARG	NE-CZ-NH1	-12.74	108.76	121.50
1	A	246	ALA	O-C-N	12.68	135.56	122.12
1	A	626	HIS	CB-CG-CD2	-11.66	116.04	131.20
1	A	576	ARG	NE-CZ-NH2	-10.99	109.31	119.20
1	A	457	SER	CB-CA-C	-10.90	100.63	110.44
1	B	643	LEU	CA-C-N	-10.85	108.25	122.79
1	B	643	LEU	C-N-CA	-10.85	108.25	122.79
1	B	224	MET	CG-SD-CE	-10.59	77.59	100.90
1	A	245	PRO	O-C-N	-10.59	108.35	122.64
1	A	646	ARG	NE-CZ-NH2	-10.49	109.76	119.20
1	A	245	PRO	N-CA-C	9.87	132.81	112.47
1	B	568	ARG	NE-CZ-NH1	9.04	130.54	121.50
1	A	599	ARG	NE-CZ-NH1	8.99	130.49	121.50
1	A	544	ARG	NE-CZ-NH2	8.95	127.26	119.20
1	B	643	LEU	O-C-N	-8.70	113.00	123.27
1	A	245	PRO	CA-C-O	8.39	135.87	120.60
1	A	626	HIS	ND1-CG-CD2	8.38	114.48	106.10
1	A	546	ARG	NE-CZ-NH1	8.27	129.77	121.50
1	A	646	ARG	NE-CZ-NH1	8.06	129.56	121.50
1	A	546	ARG	NH1-CZ-NH2	-8.02	108.87	119.30
1	A	576	ARG	CD-NE-CZ	-7.97	113.23	124.40
1	A	457	SER	CA-C-N	-7.91	110.58	119.28
1	A	457	SER	C-N-CA	-7.91	110.58	119.28
1	A	245	PRO	CA-N-CD	7.75	122.86	112.00
1	A	626	HIS	CG-ND1-CE1	-7.74	96.15	109.30
1	B	77	ARG	CD-NE-CZ	7.73	135.22	124.40
1	A	626	HIS	ND1-CE1-NE2	7.67	116.07	108.40
1	A	546	ARG	CD-NE-CZ	7.57	135.00	124.40
1	A	576	ARG	CG-CD-NE	-7.45	95.61	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	ALA	CA-C-N	-7.32	109.18	120.31
1	A	246	ALA	C-N-CA	-7.32	109.18	120.31
1	A	245	PRO	CA-C-N	-7.28	110.40	120.38
1	A	245	PRO	C-N-CA	-7.28	110.40	120.38
1	B	203	LEU	CD1-CG-CD2	7.13	126.49	110.80
1	B	546	ARG	NE-CZ-NH1	7.12	128.62	121.50
1	A	265	ASP	CA-CB-CG	-7.06	105.54	112.60
1	A	702	VAL	N-CA-C	-7.05	96.94	107.37
1	A	568	ARG	NE-CZ-NH2	6.93	125.43	119.20
1	A	599	ARG	NE-CZ-NH2	-6.84	113.04	119.20
1	B	297	GLU	CG-CD-OE1	-6.77	102.83	118.40
1	A	587	GLN	CA-C-O	-6.71	114.33	120.50
1	A	463	ARG	CG-CD-NE	-6.52	97.67	112.00
1	B	291	GLY	CA-C-N	-6.50	112.32	121.55
1	B	291	GLY	C-N-CA	-6.50	112.32	121.55
1	A	587	GLN	N-CA-CB	-6.48	99.52	111.18
1	A	247	ASP	CA-CB-CG	6.44	119.04	112.60
1	A	247	ASP	N-CA-CB	6.25	119.97	110.28
1	B	705	PRO	CB-CA-C	-6.16	103.18	111.12
1	B	604	PHE	CA-CB-CG	6.10	119.90	113.80
1	B	620	ASP	CA-CB-CG	6.05	118.65	112.60
1	A	77	ARG	NE-CZ-NH1	6.04	127.54	121.50
1	A	370	ARG	NE-CZ-NH2	-5.99	113.81	119.20
1	B	58	ARG	CA-CB-CG	-5.96	102.18	114.10
1	A	205	VAL	CA-CB-CG1	5.88	120.39	110.40
1	A	455	ASP	O-C-N	-5.84	114.83	122.59
1	A	457	SER	N-CA-C	5.80	119.97	108.59
1	A	147	ILE	CA-CB-CG2	5.80	120.36	110.50
1	A	247	ASP	CB-CA-C	5.79	121.79	110.67
1	B	296	ASP	CA-CB-CG	-5.78	106.82	112.60
1	B	546	ARG	CB-CG-CD	5.77	124.58	111.30
1	B	544	ARG	NE-CZ-NH2	5.66	124.29	119.20
1	A	246	ALA	CA-C-O	-5.60	114.58	120.63
1	B	256	TYR	CE1-CZ-CE2	5.59	131.48	120.30
1	B	576	ARG	CD-NE-CZ	5.56	132.18	124.40
1	B	568	ARG	CD-NE-CZ	5.55	132.17	124.40
1	A	568	ARG	NH1-CZ-NH2	-5.55	112.09	119.30
1	A	241	ALA	O-C-N	-5.54	116.69	122.96
1	A	455	ASP	CB-CA-C	-5.54	99.39	110.42
1	A	293	LEU	CB-CG-CD1	5.52	127.27	110.70
1	B	699	ARG	NE-CZ-NH2	-5.50	114.25	119.20
1	B	289	VAL	CA-C-N	-5.48	112.78	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	289	VAL	C-N-CA	-5.48	112.78	122.20
1	B	644	ASP	N-CA-C	-5.46	101.35	109.11
1	B	224	MET	CB-CG-SD	-5.41	96.47	112.70
1	B	287	PRO	N-CA-C	5.41	117.30	110.70
1	B	599	ARG	NE-CZ-NH1	5.38	126.88	121.50
1	B	390	LEU	CD1-CG-CD2	-5.38	98.97	110.80
1	B	292	VAL	CA-C-N	-5.34	113.47	120.95
1	B	292	VAL	C-N-CA	-5.34	113.47	120.95
1	B	16	LYS	N-CA-CB	5.32	119.54	110.50
1	B	294	ASP	N-CA-C	5.30	122.08	110.80
1	A	507	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	456	SER	N-CA-CB	-5.28	103.45	111.15
1	B	294	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	626	HIS	CG-CD2-NE2	-5.23	101.97	107.20
1	A	701	VAL	CG1-CB-CG2	5.20	122.23	110.80
1	B	292	VAL	CA-CB-CG1	5.18	119.21	110.40
1	B	399	HIS	CB-CG-CD2	-5.18	124.47	131.20
1	B	412	HIS	N-CA-C	5.14	116.88	111.28
1	B	364	LYS	CD-CE-NZ	-5.13	95.48	111.90
1	B	265	ASP	CA-CB-CG	-5.11	107.49	112.60
1	A	364	LYS	CB-CG-CD	5.09	123.01	111.30
1	A	587	GLN	CA-C-N	-5.09	114.52	119.76
1	A	587	GLN	C-N-CA	-5.09	114.52	119.76
1	A	77	ARG	NE-CZ-NH2	-5.08	114.62	119.20
1	B	297	GLU	CG-CD-OE2	5.07	130.07	118.40
1	B	695	VAL	CA-C-O	-5.07	115.37	120.69
1	B	568	ARG	NE-CZ-NH2	-5.06	114.64	119.20
1	B	190	SER	O-C-N	5.05	128.35	122.24
1	B	544	ARG	CG-CD-NE	5.04	123.08	112.00
1	A	373	ARG	CD-NE-CZ	5.03	131.45	124.40
1	A	364	LYS	CD-CE-NZ	-5.02	95.83	111.90
1	A	243	THR	N-CA-CB	-5.01	104.14	111.20

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	ALA	Mainchain
1	A	244	PRO	Peptide
1	A	335	TYR	Sidechain
1	A	430	GLN	Sidechain
1	A	454	SER	Peptide

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Mol	Chain	Res	Type	Group
1	A	455	ASP	Mainchain
1	A	654	TYR	Sidechain
1	B	335	TYR	Sidechain
1	B	455	ASP	Mainchain
1	B	568	ARG	Sidechain
1	B	654	TYR	Sidechain
1	B	706	ALA	Peptide
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	101	1
1	B	5212	0	5102	70	1
2	A	5	0	0	0	0
2	B	5	0	0	4	0
3	A	53	0	31	0	0
3	B	53	0	31	1	0
4	A	10	0	3	0	0
4	B	10	0	3	0	0
5	A	6	0	7	0	0
5	B	6	0	8	0	0
6	A	1000	0	0	62	8
6	B	957	0	0	40	7
All	All	12529	0	10287	168	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 8.

All (168) 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:147:ILE:CB	1:B:147:ILE:CG2	1.75	1.62
1:A:147:ILE:CG2	1:A:147:ILE:CB	1.77	1.58
1:A:245:PRO:N	1:A:245:PRO:CA	1.76	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:MET:CB	1:B:224:MET:CG	1.95	1.43
1:A:245:PRO:CB	1:A:245:PRO:CG	2.02	1.38
1:B:224:MET:HE3	6:B:3930:HOH:O	1.19	1.32
1:A:702:VAL:HG22	6:A:3292:HOH:O	1.24	1.28
1:B:707:ALA:HB2	6:B:3940:HOH:O	1.12	1.28
1:A:127:ASN:HB2	6:A:3956:HOH:O	1.38	1.21
1:B:475:ARG:HD2	6:B:3438:HOH:O	1.40	1.20
1:B:206:LEU:HD22	6:B:3929:HOH:O	1.42	1.17
1:A:244:PRO:C	1:A:245:PRO:CA	2.20	1.15
1:A:475:ARG:HD2	6:A:3950:HOH:O	1.47	1.15
1:A:690:GLU:HG2	6:A:3971:HOH:O	1.46	1.14
1:B:526:ALA:N	6:B:3689:HOH:O	1.90	1.04
1:B:104:ARG:HD2	6:B:3935:HOH:O	1.56	1.03
1:B:58:ARG:HG2	6:B:3370:HOH:O	1.58	1.03
1:A:224:MET:HE3	6:A:3559:HOH:O	1.57	1.02
1:B:206:LEU:HB2	6:B:3929:HOH:O	1.59	1.02
1:A:218:GLN:HG3	6:A:3951:HOH:O	1.59	1.01
1:A:147:ILE:CG2	1:A:147:ILE:CG1	2.39	0.99
1:B:609:THR:HG21	2:B:3001:SO4:O4	1.61	0.98
1:B:206:LEU:CD2	6:B:3929:HOH:O	2.02	0.96
1:A:292:VAL:HG22	1:A:292:VAL:O	1.66	0.95
1:B:576:ARG:NH1	6:B:3639:HOH:O	1.87	0.95
1:A:639:LEU:HB3	1:A:707:ALA:CB	1.98	0.94
1:B:58:ARG:CG	6:B:3370:HOH:O	2.16	0.92
1:B:224:MET:CE	6:B:3930:HOH:O	1.85	0.92
1:A:244:PRO:O	1:A:245:PRO:HA	1.70	0.91
1:A:246:ALA:HB2	6:A:3430:HOH:O	1.69	0.90
1:B:206:LEU:CB	6:B:3929:HOH:O	2.17	0.89
1:A:626:HIS:CD2	6:A:3340:HOH:O	2.24	0.88
1:A:282:GLU:HG3	6:A:3865:HOH:O	1.72	0.88
1:B:475:ARG:CD	6:B:3438:HOH:O	2.06	0.87
1:A:702:VAL:HG23	6:A:3444:HOH:O	1.76	0.85
1:B:379:HIS:HE1	1:B:646:ARG:H	1.24	0.85
1:A:218:GLN:HG3	6:A:3927:HOH:O	1.77	0.83
1:A:218:GLN:CG	6:A:3927:HOH:O	2.26	0.83
1:A:254:THR:HG22	6:A:3549:HOH:O	1.77	0.83
1:A:639:LEU:HB3	1:A:707:ALA:HB3	1.61	0.81
1:A:475:ARG:CD	6:A:3950:HOH:O	2.14	0.80
1:A:244:PRO:O	1:A:245:PRO:CA	2.28	0.80
1:A:639:LEU:HB3	1:A:707:ALA:HB1	1.65	0.76
1:A:113:ARG:HD3	6:A:3980:HOH:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:MET:CB	1:B:224:MET:SD	2.72	0.76
1:A:422:SER:HB3	6:A:3433:HOH:O	1.86	0.75
1:B:147:ILE:CG2	1:B:147:ILE:CA	2.65	0.74
1:A:626:HIS:HE1	6:A:3248:HOH:O	1.71	0.74
1:A:472:HIS:HE1	1:A:539:GLU:OE2	1.70	0.73
1:B:472:HIS:HE1	1:B:539:GLU:OE2	1.70	0.73
1:B:147:ILE:CG2	1:B:147:ILE:CG1	2.63	0.72
1:A:243:THR:HG22	6:A:3988:HOH:O	1.87	0.72
1:B:297:GLU:OE1	6:B:3912:HOH:O	2.06	0.72
6:A:3976:HOH:O	1:B:293:LEU:HD23	1.90	0.72
1:A:218:GLN:CG	6:A:3951:HOH:O	2.27	0.72
1:A:540:ASP:OD2	1:B:472:HIS:HD2	1.73	0.71
1:A:472:HIS:HD2	1:B:540:ASP:OD2	1.74	0.70
1:A:639:LEU:O	1:A:707:ALA:CB	2.39	0.70
1:A:639:LEU:O	1:A:707:ALA:HB1	1.92	0.70
1:A:218:GLN:CD	6:A:3951:HOH:O	2.35	0.69
1:A:559:GLU:OE2	6:A:3893:HOH:O	2.11	0.69
1:A:699:ARG:NH1	6:A:3495:HOH:O	2.14	0.68
1:A:245:PRO:HB2	1:A:248:ALA:H	1.58	0.68
1:B:544:ARG:HD2	6:B:3432:HOH:O	1.93	0.67
1:A:246:ALA:CB	6:A:3430:HOH:O	2.35	0.67
1:A:292:VAL:O	1:A:292:VAL:CG2	2.42	0.67
1:A:544:ARG:NH1	6:A:3459:HOH:O	2.27	0.67
1:A:626:HIS:HD2	6:A:3340:HOH:O	1.70	0.66
1:A:579:LYS:HE3	1:A:583:ALA:O	1.96	0.66
1:A:702:VAL:CG2	6:A:3292:HOH:O	2.05	0.65
1:B:242:ALA:N	6:B:3472:HOH:O	2.31	0.64
1:A:246:ALA:HA	6:A:3468:HOH:O	1.97	0.64
1:A:218:GLN:NE2	6:A:3951:HOH:O	2.31	0.64
1:A:204:LYS:CE	6:A:3908:HOH:O	2.46	0.63
1:A:626:HIS:CE1	6:A:3248:HOH:O	2.48	0.63
1:A:245:PRO:O	1:A:246:ALA:C	2.41	0.63
1:B:544:ARG:NH1	6:B:3302:HOH:O	2.32	0.63
1:B:393:ASP:OD2	1:B:399:HIS:HE1	1.81	0.62
1:A:542:SER:OG	1:A:546:ARG:NH2	2.32	0.62
1:B:102:HIS:HD2	6:B:3250:HOH:O	1.81	0.62
1:B:296:ASP:HB2	6:B:3618:HOH:O	2.00	0.62
1:A:412:HIS:HD2	1:A:653:SER:OG	1.83	0.62
1:B:77:ARG:HD3	6:B:3272:HOH:O	2.00	0.62
1:A:707:ALA:HA	6:A:3929:HOH:O	2.01	0.61
1:B:104:ARG:CD	6:B:3935:HOH:O	2.27	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:ASP:OD1	6:A:3784:HOH:O	2.16	0.60
1:B:356:LYS:HE2	6:B:3448:HOH:O	2.01	0.60
1:A:455:ASP:HB3	6:A:3934:HOH:O	2.01	0.60
1:B:609:THR:CG2	2:B:3001:SO4:O4	2.43	0.59
1:A:16:LYS:HE3	1:A:17:ILE:H	1.68	0.59
1:A:455:ASP:CA	6:A:3934:HOH:O	2.51	0.59
1:B:475:ARG:HG2	2:B:3001:SO4:O4	2.04	0.57
1:B:153:HIS:HE1	6:B:3118:HOH:O	1.87	0.57
1:B:412:HIS:HD2	1:B:653:SER:OG	1.87	0.57
1:B:89:ASP:OD2	6:B:3928:HOH:O	2.17	0.57
1:B:147:ILE:CG2	1:B:147:ILE:HB	2.19	0.57
1:B:356:LYS:CE	6:B:3448:HOH:O	2.51	0.57
1:A:705:PRO:HG3	6:A:3268:HOH:O	2.05	0.56
1:A:455:ASP:HA	6:A:3934:HOH:O	2.06	0.56
6:A:3976:HOH:O	1:B:293:LEU:CD2	2.50	0.56
1:B:379:HIS:CE1	1:B:646:ARG:H	2.15	0.56
1:A:356:LYS:NZ	1:A:359:ASN:OD1	2.37	0.56
1:A:393:ASP:OD2	1:A:399:HIS:HE1	1.88	0.56
1:A:361:GLY:C	6:A:3425:HOH:O	2.49	0.55
1:B:707:ALA:CB	6:B:3940:HOH:O	1.97	0.55
1:A:243:THR:HG21	6:A:3312:HOH:O	2.07	0.54
1:A:646:ARG:CZ	6:A:3953:HOH:O	2.55	0.54
1:A:16:LYS:CE	1:A:17:ILE:H	2.21	0.54
1:A:282:GLU:CG	6:A:3865:HOH:O	2.41	0.54
1:A:707:ALA:CA	6:A:3929:HOH:O	2.55	0.53
1:A:104:ARG:O	6:A:3966:HOH:O	2.19	0.53
1:A:639:LEU:O	1:A:707:ALA:HB2	2.08	0.53
1:B:296:ASP:OD2	6:B:3618:HOH:O	2.18	0.53
1:A:547:HIS:HE1	6:A:3937:HOH:O	1.92	0.53
1:A:33:HIS:CE1	1:A:657:LEU:HD11	2.44	0.53
1:A:243:THR:CG2	6:A:3312:HOH:O	2.56	0.52
1:B:250:GLU:OE2	1:B:254:THR:HG21	2.10	0.52
1:A:455:ASP:CB	6:A:3934:HOH:O	2.56	0.52
1:B:289:VAL:HB	1:B:293:LEU:HD12	1.90	0.51
1:A:245:PRO:CA	1:A:245:PRO:CD	2.83	0.51
1:A:703:LYS:HB3	6:B:3593:HOH:O	2.09	0.51
1:A:446:GLN:NE2	6:A:3472:HOH:O	2.30	0.51
1:A:559:GLU:CD	6:A:3893:HOH:O	2.52	0.50
1:A:104:ARG:C	6:A:3966:HOH:O	2.55	0.50
1:B:104:ARG:NH2	6:B:3858:HOH:O	2.42	0.50
1:B:33:HIS:CE1	1:B:657:LEU:HD11	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:PRO:HG2	6:B:3938:HOH:O	2.11	0.49
1:A:204:LYS:HE2	6:A:3908:HOH:O	2.08	0.49
1:A:147:ILE:CG2	1:A:147:ILE:HG12	2.36	0.49
1:B:224:MET:HE3	1:B:224:MET:HB2	1.93	0.48
1:B:297:GLU:CG	6:B:3912:HOH:O	2.61	0.48
1:B:94:GLU:O	1:B:102:HIS:HE1	1.96	0.48
1:A:58:ARG:HD2	6:A:3377:HOH:O	2.12	0.48
1:B:224:MET:CB	1:B:224:MET:HE3	2.44	0.48
1:A:204:LYS:HG3	6:A:3675:HOH:O	2.14	0.47
1:A:463:ARG:HG2	6:B:3912:HOH:O	2.15	0.46
1:A:626:HIS:CE1	6:A:3337:HOH:O	2.67	0.46
1:A:127:ASN:CB	6:A:3956:HOH:O	2.20	0.46
1:A:245:PRO:CA	1:A:245:PRO:CG	2.72	0.46
1:A:626:HIS:HD2	1:B:296:ASP:OD1	1.98	0.46
1:B:141:ALA:HA	3:B:801:FAD:C4X	2.46	0.46
1:A:83:PRO:HD3	6:A:3703:HOH:O	2.16	0.46
1:A:546:ARG:NH2	1:A:609:THR:OG1	2.49	0.46
1:A:263:GLN:NE2	6:A:3926:HOH:O	2.42	0.45
1:A:142:MET:HG2	6:A:3003:HOH:O	2.18	0.44
1:A:395:HIS:HE1	6:A:3413:HOH:O	1.99	0.44
1:B:379:HIS:HD2	1:B:449:PRO:O	2.01	0.44
1:A:640:ALA:HB2	1:A:702:VAL:HG21	2.00	0.44
1:B:368:GLN:NE2	6:B:3948:HOH:O	2.51	0.44
1:A:218:GLN:NE2	6:A:3927:HOH:O	2.38	0.43
1:B:699:ARG:NH1	1:B:699:ARG:HB3	2.33	0.43
1:A:245:PRO:HB2	1:A:248:ALA:N	2.28	0.43
1:B:546:ARG:NE	2:B:3001:SO4:O2	2.46	0.43
1:B:293:LEU:HD23	1:B:293:LEU:HA	1.85	0.43
1:A:463:ARG:CG	6:B:3912:HOH:O	2.66	0.42
1:A:568:ARG:HH11	1:A:568:ARG:HD2	1.74	0.42
1:A:147:ILE:CG2	1:A:147:ILE:CA	2.78	0.42
1:B:297:GLU:HB3	6:B:3912:HOH:O	2.19	0.42
1:A:646:ARG:NH2	6:A:3953:HOH:O	2.53	0.42
1:B:290:ASP:OD1	1:B:290:ASP:C	2.62	0.42
1:B:59:ILE:O	1:B:90:VAL:HA	2.20	0.41
1:B:690:GLU:HG2	6:B:3401:HOH:O	2.19	0.41
1:A:699:ARG:NH2	6:A:3495:HOH:O	2.54	0.41
1:B:72:LEU:HD22	1:B:92:ILE:HD11	2.02	0.41
1:A:245:PRO:HB2	1:A:248:ALA:HB2	2.03	0.41
1:B:58:ARG:HG3	6:B:3370:HOH:O	2.03	0.40
1:B:296:ASP:CB	6:B:3618:HOH:O	2.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:GLU:HG3	6:B:3912:HOH:O	2.19	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:3325:HOH:O	6:B:3903:HOH:O[3_756]	1.62	0.58
1:A:455:ASP:OD1	1:B:642:SER:OG[2_665]	1.86	0.34
6:A:3629:HOH:O	6:B:3895:HOH:O[2_665]	1.89	0.31
6:A:3978:HOH:O	6:B:3786:HOH:O[2_665]	1.93	0.27
6:A:3787:HOH:O	6:B:3484:HOH:O[4_556]	2.11	0.09
6:A:3289:HOH:O	6:B:3902:HOH:O[3_756]	2.14	0.06
6:A:3243:HOH:O	6:B:3200:HOH:O[4_556]	2.17	0.03
6:A:3440:HOH:O	6:A:3814:HOH:O[3_756]	2.19	0.01
6:A:3472:HOH:O	6:B:3826:HOH:O[2_665]	2.19	0.01

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%)	663 (98%)	15 (2%)	0	100	100
1	B	678/721 (94%)	662 (98%)	15 (2%)	1 (0%)	48	20
All	All	1356/1442 (94%)	1325 (98%)	30 (2%)	1 (0%)	48	20

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	294	ASP

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%)	531 (99%)	3 (1%)	78	58
1	B	534/566 (94%)	531 (99%)	3 (1%)	78	58
All	All	1068/1132 (94%)	1062 (99%)	6 (1%)	78	58

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	104	ARG
1	A	247	ASP
1	B	292	VAL
1	B	294	ASP
1	B	584	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	ASN
1	A	321	ASN
1	A	395	HIS
1	A	399	HIS
1	A	412	HIS
1	A	414	GLN
1	A	430	GLN
1	A	470	GLN
1	A	472	HIS
1	A	490	GLN
1	A	495	GLN
1	A	547	HIS
1	A	554	GLN
1	A	587	GLN
1	A	626	HIS
1	B	56	ASN

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Mol	Chain	Res	Type
1	B	102	HIS
1	B	153	HIS
1	B	321	ASN
1	B	379	HIS
1	B	399	HIS
1	B	412	HIS
1	B	414	GLN
1	B	470	GLN
1	B	472	HIS
1	B	554	GLN
1	B	585	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	3002	-	4,4,4	0.88	0	6,6,6	2.21	4 (66%)
5	GOL	A	902	-	5,5,5	1.31	0	5,5,5	0.88	0
5	GOL	B	1902	-	5,5,5	0.52	0	5,5,5	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	B	801	-	58,58,58	1.25	6 (10%)	85,89,89	1.42	13 (15%)
4	BE2	B	1906	-	10,10,10	2.15	3 (30%)	13,13,13	2.55	6 (46%)
4	BE2	A	906	-	10,10,10	1.39	1 (10%)	13,13,13	2.78	7 (53%)
3	FAD	A	801	-	58,58,58	1.37	9 (15%)	85,89,89	1.29	8 (9%)
2	SO4	B	3001	-	4,4,4	0.99	0	6,6,6	2.70	4 (66%)

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	-
5	GOL	A	902	-	-	0/4/4/4	-
3	FAD	B	801	-	-	5/34/50/50	0/6/6/6
4	BE2	B	1906	-	-	0/4/4/4	0/1/1/1
4	BE2	A	906	-	-	0/4/4/4	0/1/1/1
3	FAD	A	801	-	-	6/34/50/50	0/6/6/6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1906	BE2	C1-CA	3.92	1.47	1.41
3	A	801	FAD	P-O3P	3.87	1.63	1.59
3	A	801	FAD	C4X-N5	3.62	1.38	1.30
4	B	1906	BE2	O-C	3.49	1.32	1.22
4	B	1906	BE2	OXT-C	-3.26	1.20	1.30
3	B	801	FAD	C4X-N5	2.82	1.36	1.30
4	A	906	BE2	C5-C6	2.81	1.43	1.38
3	B	801	FAD	P-O3P	2.80	1.62	1.59
3	B	801	FAD	C6-C7	-2.68	1.36	1.39
3	A	801	FAD	O4B-C1B	2.64	1.48	1.42
3	A	801	FAD	C9-C9A	-2.55	1.35	1.39
3	A	801	FAD	C8A-N9A	-2.54	1.33	1.37
3	A	801	FAD	C2A-N1A	2.53	1.38	1.33
3	B	801	FAD	O4-C4	2.49	1.28	1.23
3	B	801	FAD	O2'-C2'	2.47	1.48	1.43
3	A	801	FAD	C5B-C4B	2.45	1.58	1.51
3	A	801	FAD	C4A-N9A	-2.35	1.32	1.37
3	A	801	FAD	C9A-N10	2.21	1.45	1.41
3	B	801	FAD	C9-C8	2.19	1.42	1.39

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3001	SO4	O4-S-O2	-4.79	84.54	109.56
3	A	801	FAD	C9A-C5X-N5	-4.75	117.41	122.45
4	B	1906	BE2	C5-C6-C1	4.58	128.06	119.80
4	A	906	BE2	C4-C5-C6	-4.50	114.69	120.24
4	B	1906	BE2	C6-C1-CA	-4.47	114.43	118.96
3	B	801	FAD	C9A-C5X-N5	-4.21	117.99	122.45
4	A	906	BE2	C3-CA-C1	4.06	122.50	118.16
4	A	906	BE2	C6-C1-CA	-4.02	114.89	118.96
3	B	801	FAD	C4-C4X-N5	3.91	123.61	118.21
4	A	906	BE2	C1-CA-N	-3.27	118.11	122.68
4	B	1906	BE2	O-C-C1	-3.23	114.26	121.97
4	B	1906	BE2	CA-C1-C	3.22	125.14	121.27
4	B	1906	BE2	C4-C5-C6	-3.20	116.29	120.24
4	A	906	BE2	CA-C1-C	3.18	125.10	121.27
3	B	801	FAD	C5'-C4'-C3'	-3.15	106.28	112.22
2	A	3002	SO4	O2-S-O1	3.12	131.03	109.06
4	A	906	BE2	OXT-C-O	3.04	129.88	123.35
4	A	906	BE2	C5-C6-C1	2.99	125.20	119.80
3	A	801	FAD	C5X-N5-C4X	2.96	122.88	118.09
3	A	801	FAD	C10-C4X-N5	-2.84	119.00	124.81
3	A	801	FAD	C4'-C3'-C2'	2.84	118.30	113.57
3	B	801	FAD	C4A-N9A-C8A	2.65	108.53	105.74
2	A	3002	SO4	O3-S-O2	-2.63	95.79	109.56
3	B	801	FAD	C5X-C9A-N10	2.58	120.30	117.97
3	B	801	FAD	N3A-C4A-N9A	2.56	131.51	127.17
2	A	3002	SO4	O4-S-O2	-2.55	96.23	109.56
3	B	801	FAD	C6-C7-C8	-2.52	115.99	119.69
3	B	801	FAD	C5X-C6-C7	2.52	125.49	120.83
2	B	3001	SO4	O4-S-O1	-2.46	96.68	109.56
3	A	801	FAD	C4-C4X-N5	2.41	121.54	118.21
4	B	1906	BE2	OXT-C-O	2.39	128.49	123.35
3	B	801	FAD	C6-C5X-N5	2.38	122.39	118.44
2	A	3002	SO4	O4-S-O3	2.35	121.47	108.54
3	B	801	FAD	O4B-C4B-C3B	2.30	109.73	105.15
3	B	801	FAD	C4X-C4-N3	2.23	118.92	113.25
2	B	3001	SO4	O3-S-O2	2.19	121.01	109.56
2	B	3001	SO4	O4-S-O3	-2.17	96.56	108.54
3	B	801	FAD	O4-C4-C4X	-2.17	120.80	126.53
3	A	801	FAD	C7M-C7-C8	2.11	125.06	120.76
3	A	801	FAD	C9-C9A-N10	2.08	124.65	121.85
3	B	801	FAD	O2P-P-O1P	2.07	122.10	112.44
3	A	801	FAD	O2P-P-O1P	2.04	121.93	112.44

There are no chirality outliers.

All (11) torsion outliers are listed below:

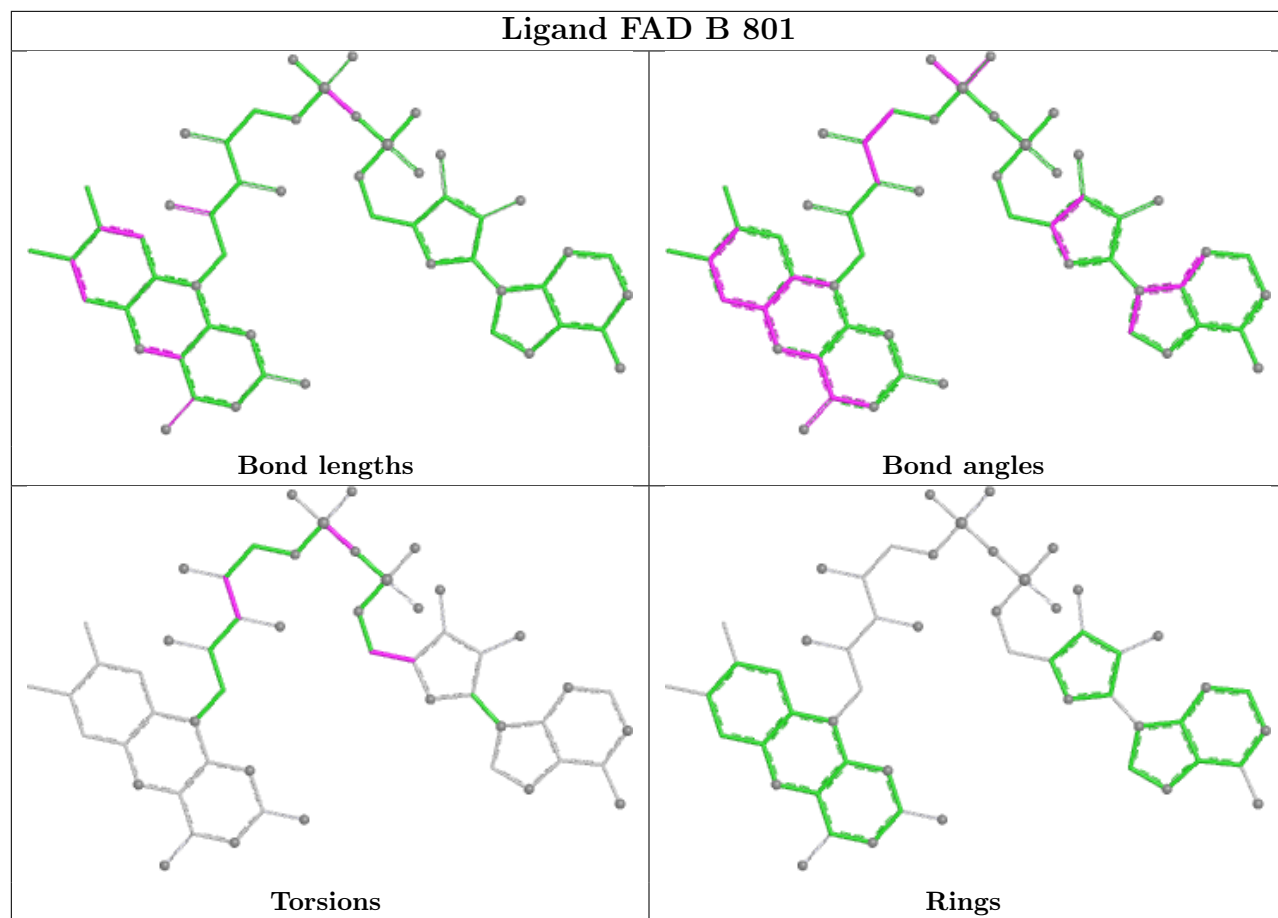
Mol	Chain	Res	Type	Atoms
3	A	801	FAD	PA-O3P-P-O5'
3	B	801	FAD	PA-O3P-P-O5'
3	A	801	FAD	C2'-C3'-C4'-O4'
3	A	801	FAD	C2'-C3'-C4'-C5'
3	B	801	FAD	O3'-C3'-C4'-O4'
3	B	801	FAD	O3'-C3'-C4'-C5'
3	A	801	FAD	O3'-C3'-C4'-O4'
3	B	801	FAD	O4B-C4B-C5B-O5B
3	A	801	FAD	O3'-C3'-C4'-C5'
3	A	801	FAD	O4B-C4B-C5B-O5B
3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

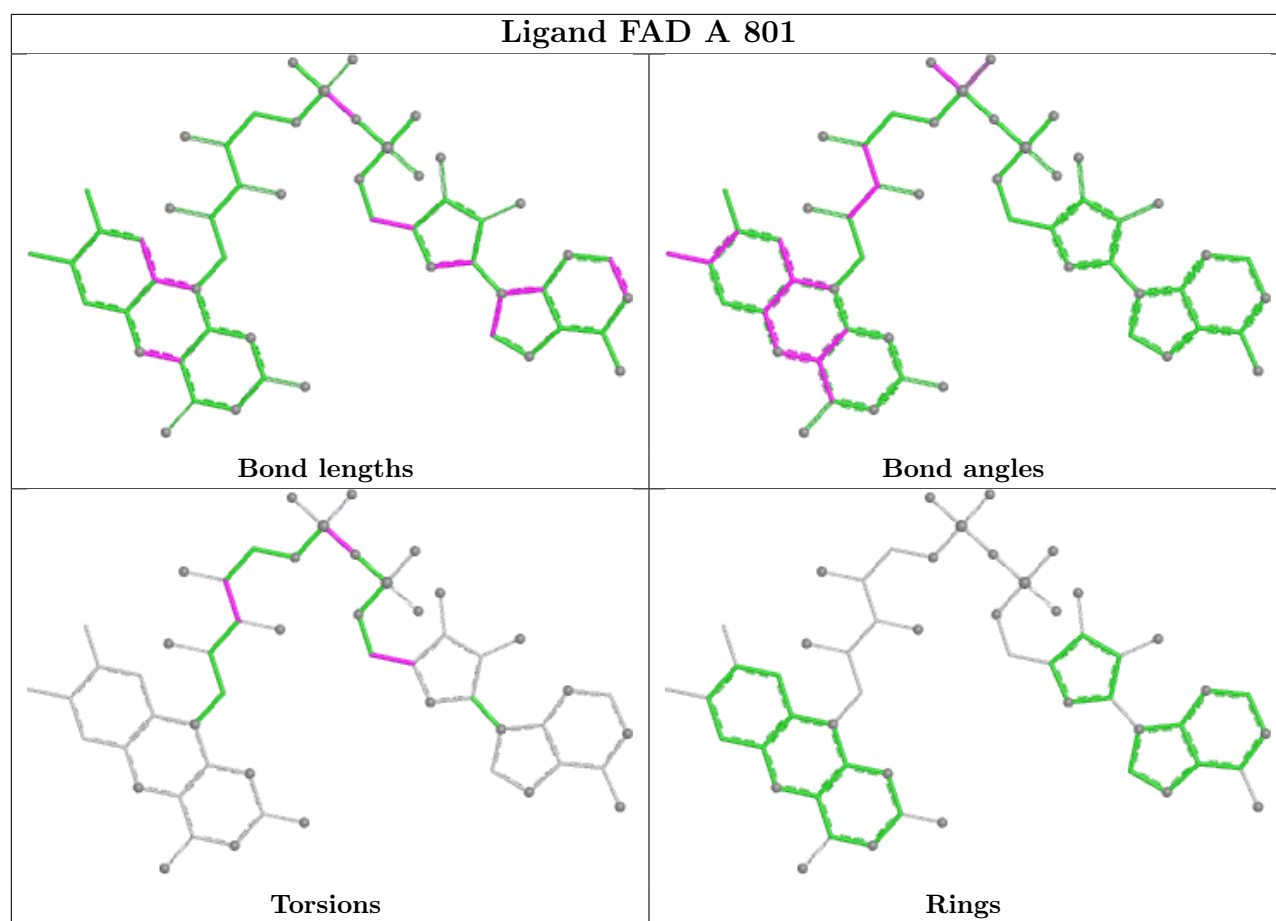
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	FAD	1	0
2	B	3001	SO4	4	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%)	-0.27	21 (3%) 51 61	8, 14, 28, 47	0
1	B	684/721 (94%)	-0.28	17 (2%) 58 68	9, 14, 29, 42	0
All	All	1368/1442 (94%)	-0.28	38 (2%) 55 64	8, 14, 29, 47	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	707	ALA	9.8
1	A	246	ALA	6.8
1	A	706	ALA	6.6
1	A	245	PRO	5.9
1	B	292	VAL	5.7
1	B	707	ALA	5.2
1	A	362	ALA	4.6
1	A	705	PRO	4.5
1	A	292	VAL	4.4
1	A	704	VAL	4.4
1	B	293	LEU	4.2
1	A	291	GLY	4.2
1	B	521	VAL	3.5
1	A	521	VAL	3.2
1	A	496	TRP	3.1
1	B	704	VAL	3.0
1	A	456	SER	2.9
1	A	104	ARG	2.9
1	A	703	LYS	2.9
1	A	132	SER	2.9
1	B	586	ALA	2.8
1	B	290	ASP	2.8
1	B	585	ASN	2.7
1	B	705	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	584	SER	2.6
1	B	291	GLY	2.6
1	B	127	ASN	2.5
1	A	243	THR	2.4
1	B	246	ALA	2.4
1	B	296	ASP	2.3
1	A	702	VAL	2.3
1	B	104	ARG	2.3
1	A	584	SER	2.1
1	A	16	LYS	2.1
1	A	455	ASP	2.1
1	B	16	LYS	2.1
1	A	127	ASN	2.1
1	B	362	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

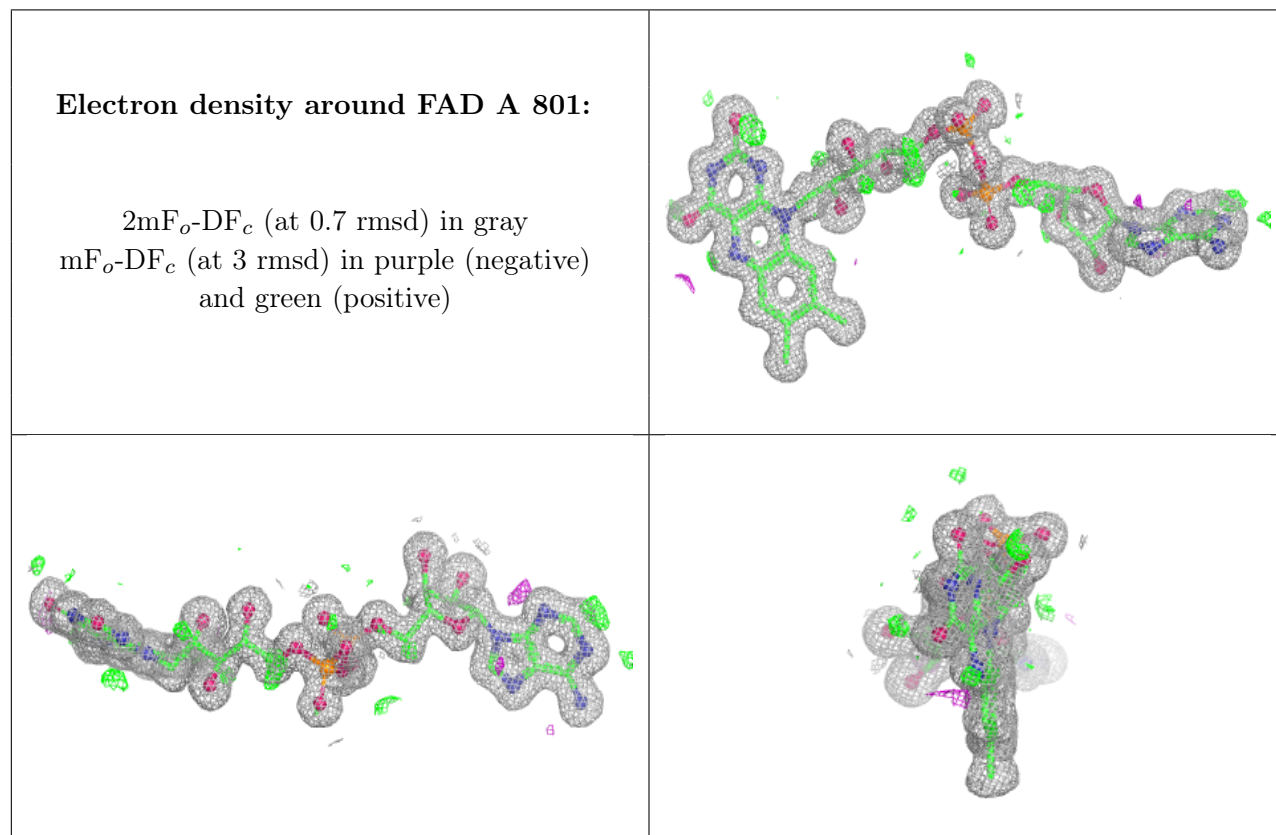
There are no oligosaccharides in this entry.

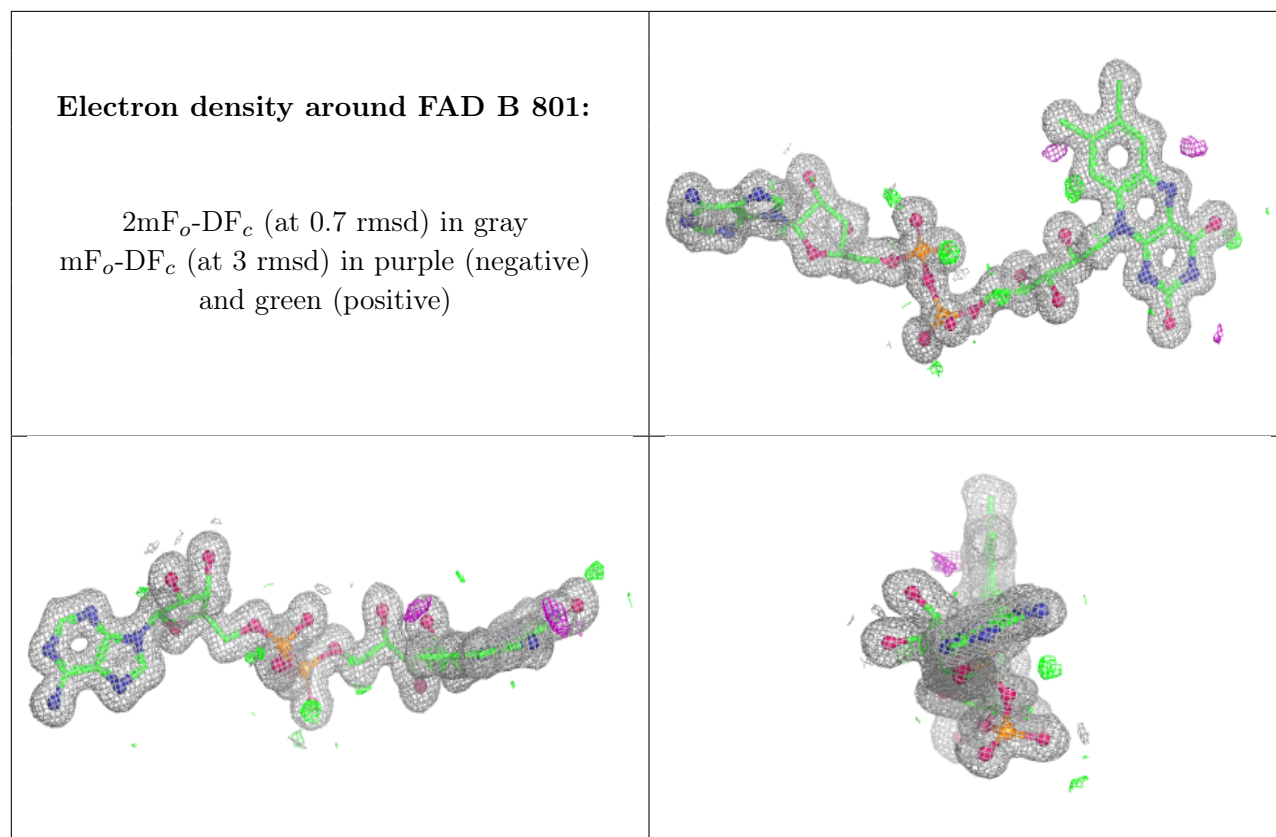
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	3002	5/5	0.96	0.09	32,36,37,43	0
2	SO4	B	3001	5/5	0.96	0.09	30,32,33,47	0
4	BE2	A	906	10/10	0.97	0.06	12,14,16,16	0
4	BE2	B	1906	10/10	0.97	0.05	13,14,16,16	0
5	GOL	B	1902	6/6	0.97	0.05	14,15,18,21	0
5	GOL	A	902	6/6	0.98	0.04	15,16,20,26	0
3	FAD	A	801	53/53	0.99	0.03	7,9,10,10	0
3	FAD	B	801	53/53	0.99	0.03	8,9,10,11	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.