



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:37 am GMT

PDB ID : 3AYJ  
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 : 1.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

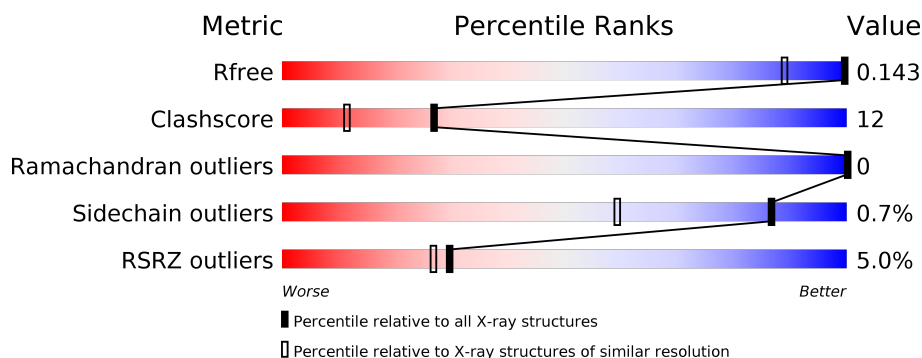
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.10 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))
$R_{free}$	100719	1192 (1.14-1.06)
Clashscore	112137	1244 (1.14-1.06)
Ramachandran outliers	110173	1198 (1.14-1.06)
Sidechain outliers	110143	1196 (1.14-1.06)
RSRZ outliers	101464	1197 (1.14-1.06)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>5%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	B	721	<div> <div>5%</div> <div> <div></div> <div>83%</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	A	3001	-	X	-	X
2	SO4	A	3002	-	X	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12913 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.

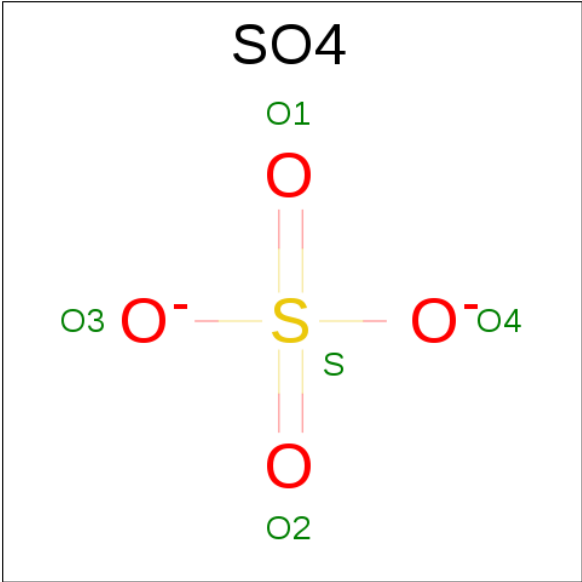
- Molecule 1 is a protein called Pro-enzyme of L-phenylalanine oxidase.

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:

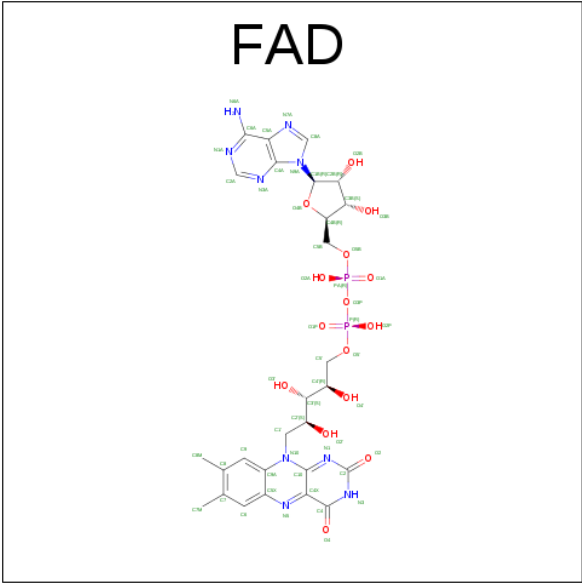
Chain	Residue	Modelled	Actual	Comment	Reference
A	714	LEU	-	EXPRESSION TAG	UNP Q5W9R9
A	715	GLU	-	EXPRESSION TAG	UNP Q5W9R9
A	716	HIS	-	EXPRESSION TAG	UNP Q5W9R9
A	717	HIS	-	EXPRESSION TAG	UNP Q5W9R9
A	718	HIS	-	EXPRESSION TAG	UNP Q5W9R9
A	719	HIS	-	EXPRESSION TAG	UNP Q5W9R9
A	720	HIS	-	EXPRESSION TAG	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: O<sub>4</sub>S).



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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



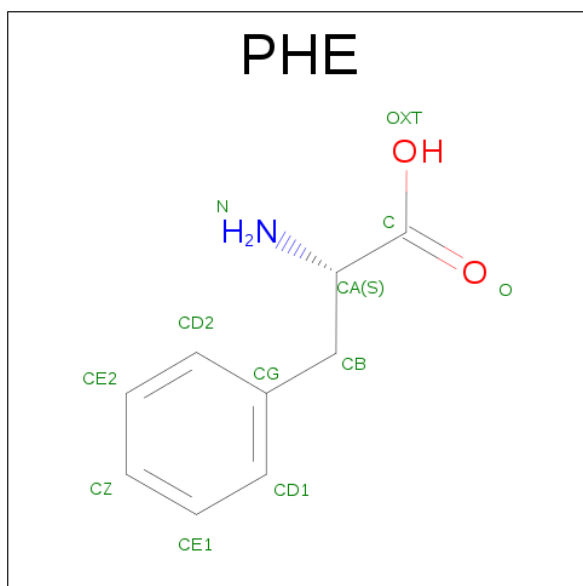
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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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 PHENYLALANINE (three-letter code: PHE) (formula:  $C_9H_{11}NO_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O		0	0
			12	9	1	2			
4	B	1	Total	C	N	O		0	0
			12	9	1	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		

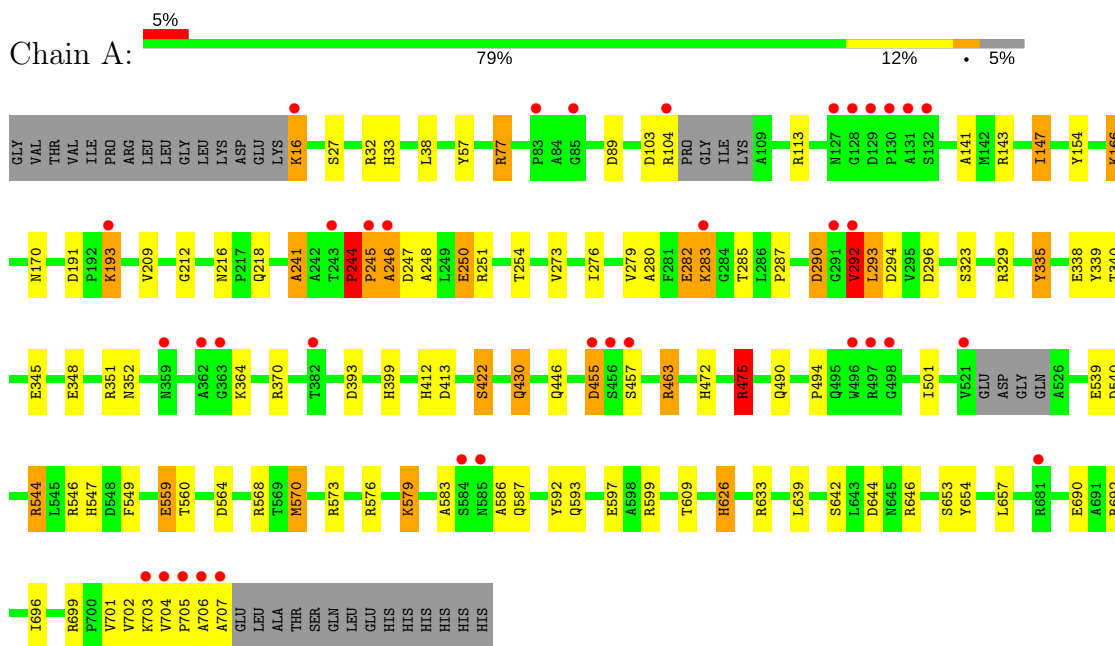
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1198	Total	O	0	0
			1198	1198		
6	B	1139	Total	O	0	0
			1139	1139		

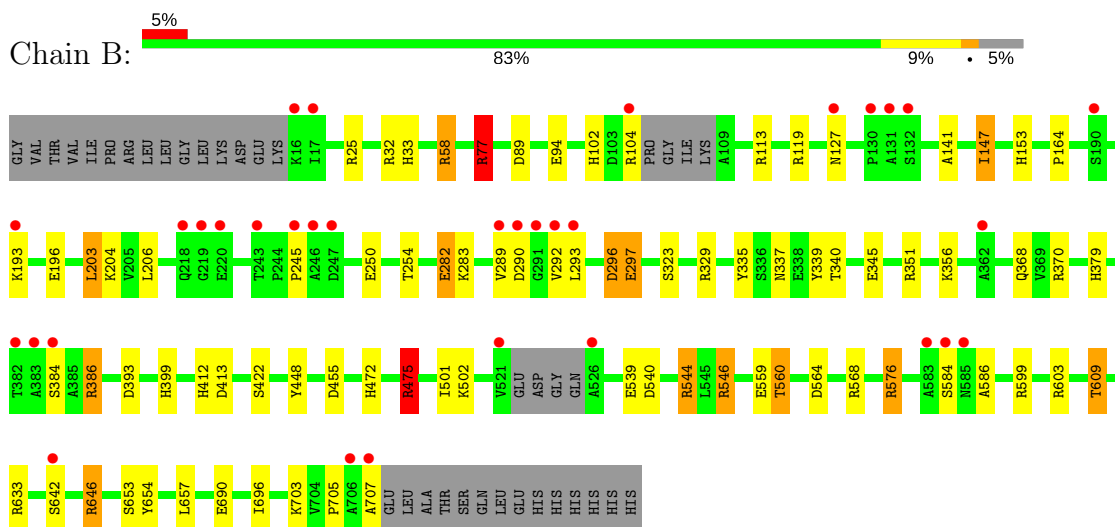
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	100.98Å 112.94Å 136.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.20 – 1.10 29.20 – 1.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.20-1.10) 98.5 (29.20-1.10)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.54 (at 1.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.111 , 0.131 0.125 , 0.143	Depositor DCC
$R_{free}$ test set	30827 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.7	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 55.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	12913	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	1.22	41/5347 (0.8%)	1.25	56/7300 (0.8%)
1	B	1.16	30/5347 (0.6%)	1.18	40/7300 (0.5%)
All	All	1.19	71/10694 (0.7%)	1.22	96/14600 (0.7%)

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

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

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	570	MET	CG-SD	-24.79	1.16	1.81
1	B	297	GLU	CD-OE2	21.54	1.49	1.25
1	B	544	ARG	CZ-NH2	-15.09	1.13	1.33
1	A	576	ARG	CZ-NH2	14.04	1.51	1.33
1	B	147	ILE	CA-CB	13.29	1.85	1.54
1	A	544	ARG	CZ-NH2	-12.16	1.17	1.33
1	B	576	ARG	CZ-NH2	12.11	1.48	1.33
1	B	544	ARG	CD-NE	10.98	1.65	1.46
1	A	323	SER	CB-OG	-10.50	1.28	1.42
1	A	147	ILE	CA-CB	10.17	1.78	1.54
1	A	422	SER	CA-CB	10.03	1.68	1.52
1	B	544	ARG	CG-CD	9.41	1.75	1.51
1	A	250	GLU	CG-CD	-9.39	1.37	1.51
1	A	544	ARG	CD-NE	9.21	1.62	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	PRO	N-CA	9.11	1.62	1.47
1	B	609	THR	CB-CG2	-9.11	1.22	1.52
1	B	296	ASP	CB-CG	8.73	1.70	1.51
1	A	32	ARG	CG-CD	-8.56	1.30	1.51
1	A	544	ARG	NE-CZ	-8.54	1.22	1.33
1	A	323	SER	CA-CB	8.24	1.65	1.52
1	B	544	ARG	NE-CZ	-8.22	1.22	1.33
1	A	246	ALA	C-O	8.01	1.38	1.23
1	A	642	SER	CB-OG	7.93	1.52	1.42
1	B	32	ARG	CG-CD	-7.81	1.32	1.51
1	A	77	ARG	CZ-NH1	-7.72	1.23	1.33
1	A	345	GLU	CG-CD	-7.71	1.40	1.51
1	A	609	THR	CB-CG2	-7.17	1.28	1.52
1	B	609	THR	CB-OG1	7.12	1.57	1.43
1	B	297	GLU	CG-CD	7.06	1.62	1.51
1	A	245	PRO	CA-C	7.06	1.67	1.52
1	A	282	GLU	CD-OE2	7.06	1.33	1.25
1	A	544	ARG	CG-CD	6.87	1.69	1.51
1	A	559	GLU	CD-OE2	-6.76	1.18	1.25
1	A	609	THR	CB-OG1	6.63	1.56	1.43
1	B	546	ARG	CZ-NH1	-6.61	1.24	1.33
1	B	282	GLU	CG-CD	6.52	1.61	1.51
1	A	597	GLU	CD-OE2	-6.43	1.18	1.25
1	A	599	ARG	NE-CZ	6.41	1.41	1.33
1	B	282	GLU	CD-OE2	6.30	1.32	1.25
1	A	154	TYR	CE2-CZ	-6.27	1.30	1.38
1	B	204	LYS	CD-CE	6.20	1.66	1.51
1	B	58	ARG	CZ-NH2	6.17	1.41	1.33
1	B	323	SER	CB-OG	-6.09	1.34	1.42
1	A	579	LYS	CD-CE	6.07	1.66	1.51
1	A	430	GLN	CD-OE1	6.07	1.37	1.24
1	B	297	GLU	CB-CG	6.00	1.63	1.52
1	A	338	GLU	CD-OE2	5.86	1.32	1.25
1	A	282	GLU	CG-CD	5.81	1.60	1.51
1	A	568	ARG	CD-NE	-5.76	1.36	1.46
1	A	57	TYR	CE1-CZ	-5.72	1.31	1.38
1	B	345	GLU	CG-CD	-5.63	1.43	1.51
1	B	502	LYS	CG-CD	5.62	1.71	1.52
1	A	27	SER	CB-OG	-5.61	1.34	1.42
1	A	283	LYS	CD-CE	5.61	1.65	1.51
1	A	245	PRO	CB-CG	5.51	1.77	1.50
1	A	283	LYS	CE-NZ	5.49	1.62	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	599	ARG	NE-CZ	5.48	1.40	1.33
1	B	559	GLU	CD-OE2	-5.39	1.19	1.25
1	B	196	GLU	CG-CD	-5.38	1.43	1.51
1	B	546	ARG	CZ-NH2	-5.29	1.26	1.33
1	A	292	VAL	CB-CG1	-5.25	1.41	1.52
1	B	560	THR	CA-CB	5.23	1.67	1.53
1	B	448	TYR	CD2-CE2	5.22	1.47	1.39
1	B	58	ARG	CZ-NH1	5.19	1.39	1.33
1	B	77	ARG	CZ-NH1	-5.19	1.26	1.33
1	A	599	ARG	CZ-NH2	-5.13	1.26	1.33
1	A	241	ALA	CA-C	5.07	1.66	1.52
1	A	626	HIS	CA-CB	5.05	1.65	1.53
1	A	339	TYR	CE2-CZ	-5.04	1.31	1.38
1	B	422	SER	CA-CB	5.02	1.60	1.52
1	A	559	GLU	CD-OE1	-5.00	1.20	1.25

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	544	ARG	NE-CZ-NH2	23.12	131.86	120.30
1	B	576	ARG	NE-CZ-NH2	20.19	130.40	120.30
1	B	544	ARG	NE-CZ-NH2	19.59	130.10	120.30
1	A	576	ARG	NE-CZ-NH2	19.37	129.99	120.30
1	A	544	ARG	NE-CZ-NH1	-18.81	110.90	120.30
1	A	599	ARG	NE-CZ-NH2	-16.92	111.84	120.30
1	A	570	MET	CG-SD-CE	16.05	125.87	100.20
1	A	576	ARG	NE-CZ-NH1	-15.94	112.33	120.30
1	B	544	ARG	NE-CZ-NH1	-15.16	112.72	120.30
1	B	386	ARG	NE-CZ-NH2	-14.53	113.03	120.30
1	A	599	ARG	NE-CZ-NH1	13.53	127.06	120.30
1	A	592	TYR	CB-CG-CD2	13.22	128.93	121.00
1	B	599	ARG	NE-CZ-NH1	12.76	126.68	120.30
1	B	77	ARG	CD-NE-CZ	12.47	141.07	123.60
1	A	692	ARG	NE-CZ-NH2	-11.71	114.44	120.30
1	B	386	ARG	NE-CZ-NH1	11.05	125.83	120.30
1	A	32	ARG	NE-CZ-NH1	10.21	125.40	120.30
1	B	576	ARG	NE-CZ-NH1	-10.12	115.24	120.30
1	A	576	ARG	CD-NE-CZ	10.10	137.74	123.60
1	B	546	ARG	NE-CZ-NH1	-10.01	115.29	120.30
1	A	247	ASP	CB-CG-OD2	9.81	127.13	118.30
1	B	599	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	A	568	ARG	NE-CZ-NH1	9.42	125.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	564	ASP	CB-CG-OD1	9.28	126.65	118.30
1	A	370	ARG	NE-CZ-NH1	9.25	124.92	120.30
1	A	559	GLU	OE1-CD-OE2	-9.04	112.45	123.30
1	B	633	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	B	297	GLU	CG-CD-OE1	-8.86	100.59	118.30
1	B	370	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	B	544	ARG	CG-CD-NE	8.30	129.23	111.80
1	A	564	ASP	CB-CG-OD1	8.25	125.72	118.30
1	A	475	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	B	370	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	B	89	ASP	CB-CG-OD1	8.10	125.59	118.30
1	A	293	LEU	CB-CG-CD1	7.90	124.43	111.00
1	A	455	ASP	CB-CG-OD1	-7.86	111.22	118.30
1	B	568	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	573	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	A	294	ASP	CB-CG-OD1	7.36	124.93	118.30
1	A	546	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	A	245	PRO	O-C-N	-7.15	111.26	122.70
1	A	247	ASP	CB-CG-OD1	-7.10	111.91	118.30
1	A	633	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	592	TYR	CB-CG-CD1	-6.98	116.81	121.00
1	A	546	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	A	77	ARG	CD-NE-CZ	6.80	133.12	123.60
1	B	89	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	B	77	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	296	ASP	CB-CG-OD1	6.74	124.37	118.30
1	A	544	ARG	CG-CD-NE	6.70	125.86	111.80
1	B	297	GLU	CG-CD-OE2	6.66	131.62	118.30
1	B	633	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	B	329	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	77	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	B	475	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	692	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	646	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	B	564	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	370	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	475	ARG	CD-NE-CZ	5.95	131.93	123.60
1	B	609	THR	OG1-CB-CG2	-5.94	96.33	110.00
1	A	463	ARG	CG-CD-NE	5.93	124.25	111.80
1	A	290	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	335	TYR	CB-CG-CD1	-5.91	117.45	121.00
1	A	609	THR	OG1-CB-CG2	-5.82	96.61	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ARG	NE-CZ-NH2	5.77	123.18	120.30
1	A	646	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	296	ASP	CB-CG-OD2	5.70	123.42	118.30
1	B	203	LEU	CB-CG-CD1	5.67	120.64	111.00
1	A	191	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	245	PRO	CA-C-O	5.65	133.76	120.20
1	A	702	VAL	O-C-N	-5.61	113.72	122.70
1	A	475	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	501	ILE	CB-CG1-CD1	5.55	129.43	113.90
1	A	364	LYS	CD-CE-NZ	-5.54	98.97	111.70
1	B	339	TYR	CB-CG-CD2	5.48	124.29	121.00
1	A	568	ARG	NH1-CZ-NH2	-5.46	113.40	119.40
1	A	166	LYS	CD-CE-NZ	5.45	124.23	111.70
1	A	573	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	546	ARG	NH1-CZ-NH2	5.41	125.34	119.40
1	B	546	ARG	NH1-CZ-NH2	5.37	125.31	119.40
1	A	549	PHE	CB-CG-CD2	5.37	124.56	120.80
1	A	329	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	A	701	VAL	CG1-CB-CG2	5.34	119.44	110.90
1	A	564	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	B	119	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	244	PRO	C-N-CD	5.26	139.44	128.40
1	B	568	ARG	CG-CD-NE	-5.22	100.83	111.80
1	B	603	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	348	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	B	25	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	89	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	692	ARG	CD-NE-CZ	5.12	130.76	123.60
1	B	546	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	702	VAL	N-CA-C	-5.07	97.31	111.00
1	B	576	ARG	NH1-CZ-NH2	-5.01	113.89	119.40

There are no chirality outliers.

All (8) 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	654	TYR	Sidechain
1	B	335	TYR	Sidechain

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Mol	Chain	Res	Type	Group
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	135	0
1	B	5212	0	5102	108	2
2	A	10	0	0	1	0
3	A	53	0	31	2	0
3	B	53	0	31	2	0
4	A	12	0	8	1	0
4	B	12	0	8	1	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	1198	0	0	96	6
6	B	1139	0	0	73	3
All	All	12913	0	10298	240	6

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 12.

All (240) 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:544:ARG:CD	1:B:544:ARG:CG	1.75	1.61
1:A:147:ILE:CA	1:A:147:ILE:CB	1.78	1.55
1:B:147:ILE:CB	1:B:147:ILE:CA	1.85	1.51
1:A:245:PRO:CG	1:A:245:PRO:CB	1.77	1.49
1:A:352:ASN:HB3	6:A:7156:HOH:O	1.16	1.32
1:B:296:ASP:HB3	6:B:5588:HOH:O	1.28	1.30
1:A:707:ALA:HA	6:A:7159:HOH:O	1.34	1.25
1:A:570:MET:SD	1:A:570:MET:CG	1.16	1.25
1:A:250:GLU:HG2	6:A:7206:HOH:O	1.36	1.22
1:B:203:LEU:CD2	6:B:7224:HOH:O	1.78	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:ARG:NH1	6:B:7215:HOH:O	1.72	1.21
1:B:58:ARG:HG2	6:B:6553:HOH:O	1.38	1.21
1:B:707:ALA:HB2	6:B:7262:HOH:O	1.42	1.20
1:B:707:ALA:HB1	6:B:7180:HOH:O	1.05	1.19
1:B:609:THR:HG22	6:B:7205:HOH:O	1.39	1.19
1:A:276:ILE:HG21	6:A:7337:HOH:O	1.43	1.18
1:A:690:GLU:HG3	6:A:7212:HOH:O	1.02	1.17
1:B:290:ASP:OD1	1:B:292:VAL:HG22	1.45	1.16
1:A:570:MET:SD	1:A:570:MET:CB	2.35	1.12
1:A:475:ARG:HD2	6:A:7220:HOH:O	1.46	1.12
1:A:570:MET:SD	1:A:570:MET:HG3	1.73	1.12
1:B:475:ARG:HD2	6:B:5680:HOH:O	1.47	1.12
1:A:570:MET:SD	1:A:570:MET:HG2	1.73	1.10
1:B:164:PRO:HG2	6:B:6342:HOH:O	1.51	1.10
1:A:273:VAL:HG21	6:A:7335:HOH:O	0.92	1.09
1:B:475:ARG:CD	6:B:5680:HOH:O	1.97	1.09
1:B:356:LYS:HE2	6:B:7124:HOH:O	1.52	1.08
1:B:206:LEU:HD22	6:B:7164:HOH:O	1.52	1.08
1:B:282:GLU:HG3	6:B:6095:HOH:O	1.53	1.07
1:A:475:ARG:CD	6:A:7220:HOH:O	2.01	1.06
1:B:203:LEU:HD23	6:B:7224:HOH:O	1.49	1.00
1:B:203:LEU:HD22	6:B:7224:HOH:O	1.51	0.98
1:B:368:GLN:CD	6:B:7218:HOH:O	2.04	0.96
1:A:282:GLU:HG3	6:A:6123:HOH:O	1.64	0.96
1:B:104:ARG:HD2	6:B:7126:HOH:O	1.65	0.95
1:A:250:GLU:OE1	6:A:6445:HOH:O	1.85	0.94
1:A:276:ILE:HD13	6:A:7337:HOH:O	1.67	0.94
1:A:218:GLN:HG3	6:A:7172:HOH:O	1.68	0.93
1:B:379:HIS:HE1	1:B:646:ARG:H	1.15	0.93
1:A:250:GLU:CG	6:A:7206:HOH:O	2.02	0.93
1:B:707:ALA:CB	6:B:7180:HOH:O	1.74	0.92
1:A:707:ALA:HB1	6:A:5379:HOH:O	1.70	0.91
1:A:283:LYS:HB3	6:A:7314:HOH:O	1.69	0.90
1:B:104:ARG:CD	6:B:7126:HOH:O	2.17	0.89
1:B:206:LEU:CD2	6:B:7164:HOH:O	2.13	0.89
1:B:292:VAL:HB	6:B:7240:HOH:O	1.72	0.89
1:B:283:LYS:HG3	6:B:5754:HOH:O	1.72	0.89
1:B:58:ARG:CG	6:B:6553:HOH:O	2.07	0.84
1:B:290:ASP:OD1	1:B:292:VAL:CG2	2.25	0.83
1:B:290:ASP:CG	1:B:292:VAL:HG22	1.99	0.83
1:A:706:ALA:O	1:A:707:ALA:HB2	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ARG:HD3	6:B:6119:HOH:O	1.79	0.82
1:A:699:ARG:HD2	6:A:7210:HOH:O	1.79	0.82
1:A:703:LYS:O	6:A:7160:HOH:O	1.99	0.81
1:A:147:ILE:CA	1:A:147:ILE:CG1	2.58	0.80
6:A:6724:HOH:O	1:B:293:LEU:HD23	1.82	0.78
1:A:254:THR:HG21	6:A:6445:HOH:O	1.82	0.78
1:A:280:ALA:O	6:A:7314:HOH:O	1.99	0.78
1:A:351:ARG:HD3	6:A:6414:HOH:O	1.84	0.78
1:A:340:THR:HG21	6:A:6343:HOH:O	1.86	0.75
1:B:77:ARG:HD3	6:B:5420:HOH:O	1.86	0.75
1:A:705:PRO:O	6:A:7176:HOH:O	2.05	0.75
1:B:340:THR:HG21	6:B:6217:HOH:O	1.87	0.74
1:A:113:ARG:NH2	6:A:7163:HOH:O	2.19	0.74
1:A:279:VAL:HG12	6:A:7325:HOH:O	1.87	0.74
1:A:705:PRO:CB	6:A:7245:HOH:O	2.35	0.74
1:B:560:THR:HG22	6:B:7165:HOH:O	1.88	0.74
1:A:413:ASP:HB3	6:A:7191:HOH:O	1.87	0.73
1:A:147:ILE:CA	1:A:147:ILE:CG2	2.66	0.73
1:A:639:LEU:O	1:A:707:ALA:HB3	1.89	0.73
1:A:250:GLU:HG2	6:A:6445:HOH:O	1.89	0.72
1:A:193:LYS:HD2	6:A:5998:HOH:O	1.89	0.72
1:A:540:ASP:OD2	1:B:472:HIS:HD2	1.72	0.71
1:B:475:ARG:HD3	6:B:5680:HOH:O	1.74	0.71
1:A:705:PRO:HD3	6:A:7108:HOH:O	1.90	0.71
1:B:147:ILE:CA	1:B:147:ILE:HD13	2.19	0.71
1:B:147:ILE:CG1	1:B:147:ILE:CA	2.69	0.71
1:A:457:SER:OG	1:B:292:VAL:HG21	1.90	0.71
1:A:472:HIS:HE1	1:A:539:GLU:OE2	1.73	0.70
1:A:285:THR:OG1	6:A:7314:HOH:O	2.10	0.70
1:B:472:HIS:HE1	1:B:539:GLU:OE2	1.74	0.70
1:B:544:ARG:CB	1:B:544:ARG:CD	2.68	0.70
1:B:283:LYS:HE2	6:B:7034:HOH:O	1.91	0.70
1:A:472:HIS:HD2	1:B:540:ASP:OD2	1.74	0.70
1:A:559:GLU:OE2	6:A:7204:HOH:O	2.09	0.70
1:A:705:PRO:HG3	6:A:5548:HOH:O	1.91	0.69
1:B:609:THR:CB	6:B:7205:HOH:O	2.36	0.69
1:B:297:GLU:OE1	6:B:6929:HOH:O	2.10	0.69
1:B:254:THR:HG22	6:B:6718:HOH:O	1.92	0.69
1:A:104:ARG:HD2	1:A:104:ARG:C	2.13	0.69
1:B:206:LEU:CB	6:B:7164:HOH:O	2.41	0.69
1:A:704:VAL:HG11	6:A:7291:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:SER:CB	1:B:292:VAL:HG21	2.23	0.69
1:A:475:ARG:HD3	6:A:7220:HOH:O	1.82	0.68
1:A:38:LEU:O	6:A:5838:HOH:O	2.11	0.68
1:A:644:ASP:OD1	6:A:6812:HOH:O	2.11	0.68
1:B:544:ARG:NH1	6:B:7202:HOH:O	2.26	0.68
1:B:696:ILE:HD11	6:B:6208:HOH:O	1.91	0.68
1:B:584:SER:O	6:B:7278:HOH:O	2.11	0.67
1:B:104:ARG:CG	6:B:7126:HOH:O	2.38	0.67
1:A:254:THR:HG22	6:A:6005:HOH:O	1.94	0.67
1:B:340:THR:CG2	6:B:6217:HOH:O	2.41	0.67
1:A:422:SER:HB3	6:A:5596:HOH:O	1.94	0.66
1:B:147:ILE:HD13	1:B:147:ILE:HA	1.77	0.66
1:A:570:MET:SD	1:A:570:MET:CA	2.83	0.66
1:B:290:ASP:O	6:B:6146:HOH:O	2.13	0.66
1:A:639:LEU:O	1:A:707:ALA:CB	2.44	0.66
1:A:244:PRO:O	6:A:6974:HOH:O	2.13	0.66
1:B:206:LEU:HB2	6:B:7164:HOH:O	1.94	0.66
1:A:455:ASP:OD1	6:A:7148:HOH:O	2.14	0.65
1:A:570:MET:CE	1:A:570:MET:CG	2.65	0.65
1:A:544:ARG:NH1	6:A:5439:HOH:O	2.30	0.65
1:B:455:ASP:OD2	6:B:7158:HOH:O	2.15	0.64
1:A:412:HIS:HD2	1:A:653:SER:OG	1.81	0.64
1:B:393:ASP:OD2	1:B:399:HIS:HE1	1.80	0.64
1:A:706:ALA:HA	6:A:7160:HOH:O	1.96	0.64
1:A:706:ALA:O	1:A:707:ALA:CB	2.43	0.63
1:B:147:ILE:CD1	1:B:147:ILE:CA	2.75	0.63
1:B:379:HIS:CE1	1:B:646:ARG:H	2.07	0.63
1:B:203:LEU:CB	6:B:7224:HOH:O	2.47	0.63
1:B:250:GLU:OE2	1:B:254:THR:HG21	1.99	0.63
3:B:801:FAD:N5	4:B:1904:PHE:HA	2.13	0.62
1:B:104:ARG:HA	6:B:6710:HOH:O	1.99	0.62
1:A:250:GLU:CG	6:A:6445:HOH:O	2.46	0.62
1:A:455:ASP:HB2	6:A:7170:HOH:O	1.99	0.62
1:A:703:LYS:C	6:A:7160:HOH:O	2.38	0.62
1:B:412:HIS:HD2	1:B:653:SER:OG	1.82	0.62
1:A:413:ASP:CB	6:A:7191:HOH:O	2.43	0.61
1:A:147:ILE:CA	1:A:147:ILE:HD13	2.31	0.61
1:A:393:ASP:OD2	1:A:399:HIS:HE1	1.82	0.61
1:B:102:HIS:HD2	6:B:5647:HOH:O	1.83	0.61
1:A:251:ARG:CD	6:A:7310:HOH:O	2.49	0.61
1:A:193:LYS:N	1:A:193:LYS:HD3	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ASN:ND2	6:B:7247:HOH:O	2.32	0.60
1:B:153:HIS:HE1	6:B:5244:HOH:O	1.83	0.60
1:B:193:LYS:NZ	6:B:6826:HOH:O	2.32	0.60
1:B:609:THR:CG2	6:B:7205:HOH:O	2.14	0.59
1:B:113:ARG:HD2	6:B:6723:HOH:O	2.02	0.59
1:A:147:ILE:CA	1:A:147:ILE:CD1	2.80	0.59
1:B:290:ASP:HB3	6:B:6327:HOH:O	2.03	0.59
1:A:705:PRO:CA	6:A:7245:HOH:O	2.51	0.59
1:A:147:ILE:HA	1:A:147:ILE:HD13	1.85	0.58
1:B:368:GLN:CG	6:B:7218:HOH:O	2.46	0.58
1:A:218:GLN:CG	6:A:7172:HOH:O	2.40	0.58
1:A:212:GLY:HA3	6:A:7337:HOH:O	2.02	0.58
1:B:282:GLU:CG	6:B:6095:HOH:O	2.30	0.58
1:A:626:HIS:HE1	6:A:5396:HOH:O	1.87	0.58
3:A:801:FAD:N5	4:A:904:PHE:HA	2.20	0.57
1:A:340:THR:CG2	6:A:6343:HOH:O	2.51	0.57
1:B:384:SER:HA	6:B:7129:HOH:O	2.05	0.57
6:A:6724:HOH:O	1:B:293:LEU:CD2	2.46	0.57
1:A:209:VAL:HA	6:A:7337:HOH:O	2.05	0.57
1:A:147:ILE:O	1:A:147:ILE:HG22	2.05	0.56
1:A:455:ASP:CA	6:A:7170:HOH:O	2.54	0.56
1:B:544:ARG:HD2	6:B:5592:HOH:O	2.05	0.55
1:A:494:PRO:HG2	1:A:501:ILE:HG13	1.89	0.55
1:A:593:GLN:HG3	6:A:7265:HOH:O	2.07	0.55
1:A:147:ILE:C	1:A:147:ILE:CB	2.69	0.55
1:A:218:GLN:NE2	6:A:7172:HOH:O	2.39	0.55
1:A:696:ILE:HD11	6:A:6293:HOH:O	2.07	0.54
1:A:77:ARG:NH1	6:A:7017:HOH:O	2.25	0.54
1:A:147:ILE:CB	1:A:147:ILE:N	2.63	0.53
1:A:455:ASP:HA	6:A:7170:HOH:O	2.07	0.53
1:A:703:LYS:HD3	6:A:6932:HOH:O	2.07	0.53
1:A:455:ASP:CB	6:A:7087:HOH:O	2.56	0.53
1:B:104:ARG:HG2	6:B:7126:HOH:O	2.03	0.53
1:B:368:GLN:HG2	6:B:7218:HOH:O	2.04	0.53
1:B:703:LYS:O	6:B:7238:HOH:O	2.19	0.53
1:A:290:ASP:HB3	1:A:292:VAL:CG1	2.38	0.52
1:B:94:GLU:O	1:B:102:HIS:HE1	1.92	0.52
1:A:413:ASP:HB3	6:B:6934:HOH:O	2.08	0.52
1:B:368:GLN:NE2	6:B:6190:HOH:O	2.42	0.52
1:A:246:ALA:HA	6:A:6536:HOH:O	2.10	0.51
1:A:251:ARG:HD3	6:A:7310:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ASP:HB3	6:A:7087:HOH:O	2.09	0.51
1:B:147:ILE:CG2	1:B:147:ILE:CA	2.80	0.51
1:A:103:ASP:O	1:A:104:ARG:HB3	2.12	0.50
1:A:544:ARG:HD2	6:A:5514:HOH:O	2.12	0.50
1:A:33:HIS:CE1	1:A:657:LEU:HD11	2.46	0.50
1:A:547:HIS:HE1	6:A:5990:HOH:O	1.93	0.50
1:B:147:ILE:CB	1:B:147:ILE:N	2.68	0.50
1:B:141:ALA:HA	3:B:801:FAD:C4X	2.42	0.49
1:A:77:ARG:HD3	6:A:7017:HOH:O	2.12	0.49
1:A:218:GLN:CD	6:A:7172:HOH:O	2.48	0.49
1:B:292:VAL:HA	6:B:7229:HOH:O	2.12	0.49
1:B:546:ARG:HH11	1:B:546:ARG:CG	2.26	0.49
1:A:245:PRO:HB2	1:A:248:ALA:HB2	1.94	0.49
1:A:586:ALA:N	6:A:7232:HOH:O	2.45	0.49
1:A:292:VAL:HA	6:A:7166:HOH:O	2.11	0.49
1:A:626:HIS:HD2	6:B:5588:HOH:O	1.94	0.49
1:A:446:GLN:HG3	6:A:7233:HOH:O	2.13	0.49
1:A:705:PRO:CD	6:A:7108:HOH:O	2.54	0.48
1:A:579:LYS:HE3	1:A:583:ALA:O	2.14	0.47
1:A:216:ASN:OD1	6:A:6101:HOH:O	2.20	0.47
1:B:290:ASP:OD2	1:B:292:VAL:HG22	2.15	0.47
1:B:33:HIS:CE1	1:B:657:LEU:HD11	2.49	0.47
1:B:586:ALA:N	6:B:7278:HOH:O	2.33	0.47
1:A:457:SER:HB2	1:B:292:VAL:HG11	1.98	0.46
1:A:705:PRO:HB2	6:A:7245:HOH:O	2.10	0.46
1:A:141:ALA:HA	3:A:801:FAD:C4X	2.45	0.46
1:A:245:PRO:HA	6:A:6002:HOH:O	2.16	0.45
1:A:351:ARG:CD	6:A:6414:HOH:O	2.53	0.45
1:A:104:ARG:O	6:A:6534:HOH:O	2.21	0.45
1:A:16:LYS:N	6:A:7308:HOH:O	2.50	0.45
1:A:490:GLN:NE2	6:A:7168:HOH:O	2.49	0.44
6:A:7125:HOH:O	1:B:586:ALA:HB3	2.17	0.44
1:A:560:THR:HG22	6:A:7274:HOH:O	2.16	0.44
1:A:245:PRO:HB2	1:A:248:ALA:CB	2.47	0.44
1:A:218:GLN:HG3	6:A:7035:HOH:O	2.18	0.44
1:B:104:ARG:HG2	6:B:7008:HOH:O	2.18	0.44
1:A:290:ASP:HB3	1:A:292:VAL:HG12	1.98	0.44
1:A:626:HIS:CD2	6:A:5999:HOH:O	2.71	0.44
1:B:351:ARG:CD	6:B:6119:HOH:O	2.51	0.43
1:B:104:ARG:CA	6:B:6710:HOH:O	2.63	0.43
1:A:587:GLN:NE2	6:A:7192:HOH:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:PRO:C	6:A:7160:HOH:O	2.56	0.43
1:B:292:VAL:HG23	1:B:293:LEU:N	2.34	0.43
6:A:7254:HOH:O	1:B:413:ASP:HB3	2.19	0.43
1:A:166:LYS:NZ	6:A:6891:HOH:O	2.51	0.43
1:A:218:GLN:CG	6:A:7035:HOH:O	2.66	0.43
1:A:287:PRO:HA	6:A:7333:HOH:O	2.18	0.43
1:A:705:PRO:O	6:A:7160:HOH:O	2.22	0.43
1:B:297:GLU:CG	6:B:6929:HOH:O	2.66	0.42
1:B:690:GLU:HG2	6:B:5804:HOH:O	2.19	0.42
1:B:245:PRO:HG2	6:B:6569:HOH:O	2.18	0.42
1:B:164:PRO:CG	6:B:6342:HOH:O	2.31	0.42
1:A:293:LEU:O	6:A:7169:HOH:O	2.22	0.42
1:B:705:PRO:HG2	6:B:7020:HOH:O	2.19	0.41
1:A:273:VAL:CG2	6:A:7335:HOH:O	1.83	0.41
1:A:626:HIS:CE1	6:A:5784:HOH:O	2.72	0.41
1:B:289:VAL:HB	1:B:293:LEU:HD12	2.02	0.41
1:B:297:GLU:HG3	6:B:6929:HOH:O	2.20	0.41
1:B:337:ASN:ND2	6:B:5923:HOH:O	2.54	0.41
1:A:706:ALA:C	6:A:7176:HOH:O	2.59	0.41
1:B:147:ILE:CB	1:B:147:ILE:C	2.76	0.41
1:B:546:ARG:HH11	1:B:546:ARG:HG3	1.85	0.41
1:B:193:LYS:CE	6:B:5724:HOH:O	2.68	0.40
1:A:143:ARG:HH11	1:A:170:ASN:HD21	1.69	0.40
2:A:3001:SO4:O4	1:B:546:ARG:NE	2.50	0.40
1:A:412:HIS:CD2	1:A:653:SER:OG	2.69	0.40

All (6) 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:6708:HOH:O	6:B:5918:HOH:O[3_756]	1.53	0.67
1:B:642:SER:O	6:A:7291:HOH:O[2_664]	1.63	0.57
6:A:5893:HOH:O	6:B:5532:HOH:O[3_756]	1.66	0.54
6:A:5408:HOH:O	6:B:6743:HOH:O[2_664]	1.70	0.50
1:B:642:SER:C	6:A:7291:HOH:O[2_664]	1.98	0.22
6:A:5935:HOH:O	6:A:7149:HOH:O[3_756]	2.14	0.06

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	678/721 (94%)	662 (98%)	16 (2%)	0	100	100
1	B	678/721 (94%)	661 (98%)	17 (2%)	0	100	100
All	All	1356/1442 (94%)	1323 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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%)	529 (99%)	5 (1%)	82	51
1	B	534/566 (94%)	532 (100%)	2 (0%)	93	77
All	All	1068/1132 (94%)	1061 (99%)	7 (1%)	87	59

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	193	LYS
1	A	292	VAL
1	A	463	ARG
1	A	475	ARG
1	B	386	ARG
1	B	475	ARG

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	170	ASN
1	A	216	ASN
1	A	399	HIS
1	A	412	HIS
1	A	446	GLN
1	A	472	HIS
1	A	547	HIS
1	A	587	GLN
1	A	626	HIS
1	B	102	HIS
1	B	127	ASN
1	B	153	HIS
1	B	337	ASN
1	B	379	HIS
1	B	399	HIS
1	B	412	HIS
1	B	472	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	3001	-	4,4,4	1.02	0	6,6,6	3.53	4 (66%)
2	SO4	A	3002	-	4,4,4	0.99	0	6,6,6	3.11	2 (33%)
3	FAD	A	801	-	51,58,58	1.14	4 (7%)	54,89,89	1.95	7 (12%)
5	GOL	A	902	-	5,5,5	0.88	0	5,5,5	0.65	0
4	PHE	A	904	-	8,12,12	0.81	0	10,15,15	0.49	0
5	GOL	B	1902	-	5,5,5	0.79	0	5,5,5	0.53	0
4	PHE	B	1904	-	8,12,12	0.80	0	10,15,15	0.53	0
3	FAD	B	801	-	51,58,58	1.28	6 (11%)	54,89,89	1.64	6 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	3001	-	-	0/0/0/0	0/0/0/0
2	SO4	A	3002	-	-	0/0/0/0	0/0/0/0
3	FAD	A	801	-	-	0/28/50/50	0/6/6/6
5	GOL	A	902	-	-	0/4/4/4	0/0/0/0
4	PHE	A	904	-	-	0/4/8/8	0/1/1/1
5	GOL	B	1902	-	-	0/4/4/4	0/0/0/0
4	PHE	B	1904	-	-	0/4/8/8	0/1/1/1
3	FAD	B	801	-	-	0/28/50/50	0/6/6/6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	FAD	C4-C4X	-3.05	1.35	1.41
3	B	801	FAD	C8A-N7A	-2.81	1.29	1.34
3	A	801	FAD	C4-C4X	-2.32	1.37	1.41
3	A	801	FAD	C8A-N7A	-2.19	1.30	1.34
3	B	801	FAD	C9A-N10	2.15	1.41	1.38
3	A	801	FAD	C4-N3	2.84	1.38	1.33
3	A	801	FAD	C4X-N5	2.95	1.37	1.33
3	B	801	FAD	C4-N3	3.00	1.38	1.33
3	B	801	FAD	O4B-C1B	3.02	1.45	1.41
3	B	801	FAD	C4X-N5	3.07	1.37	1.33

All (19) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	SO4	O4-S-O1	-5.07	81.28	109.26
2	A	3002	SO4	O3-S-O2	-4.88	82.38	109.26
3	A	801	FAD	C4X-C4-N3	-4.42	117.19	123.48
2	A	3001	SO4	O3-S-O1	-4.38	85.11	109.26
3	A	801	FAD	C4X-C10-N10	-3.37	118.18	120.52
3	B	801	FAD	C4X-C4-N3	-3.24	118.88	123.48
3	A	801	FAD	C4-C4X-C10	-2.27	118.13	119.96
3	B	801	FAD	C4A-C5A-N7A	2.05	111.39	109.41
3	B	801	FAD	C4X-N5-C5X	2.25	119.14	116.76
3	A	801	FAD	C6-C5X-N5	2.31	121.68	118.97
3	A	801	FAD	C1'-N10-C9A	2.75	120.87	118.35
3	A	801	FAD	C4X-N5-C5X	2.80	119.72	116.76
3	B	801	FAD	C6-C5X-N5	3.11	122.61	118.97
2	A	3001	SO4	O4-S-O3	3.40	124.28	108.96
2	A	3001	SO4	O4-S-O2	3.59	129.07	109.26
3	B	801	FAD	C1'-N10-C9A	3.85	121.87	118.35
2	A	3002	SO4	O2-S-O1	5.33	146.94	109.64
3	B	801	FAD	C4-N3-C2	7.46	121.68	115.16
3	A	801	FAD	C4-N3-C2	10.14	124.03	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3001	SO4	1	0
3	A	801	FAD	2	0
4	A	904	PHE	1	0
4	B	1904	PHE	1	0
3	B	801	FAD	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	684/721 (94%)	-0.03	36 (5%) 27 25	7, 12, 25, 44	0
1	B	684/721 (94%)	-0.06	33 (4%) 31 28	8, 13, 26, 39	0
All	All	1368/1442 (94%)	-0.04	69 (5%) 30 27	7, 13, 25, 44	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	707	ALA	11.9
1	B	292	VAL	9.6
1	A	706	ALA	8.6
1	A	362	ALA	8.2
1	A	104	ARG	8.1
1	A	521	VAL	6.8
1	A	704	VAL	6.2
1	B	707	ALA	6.2
1	A	131	ALA	6.1
1	B	293	LEU	6.0
1	B	521	VAL	5.9
1	A	132	SER	5.8
1	A	246	ALA	5.6
1	A	705	PRO	5.3
1	A	128	GLY	5.3
1	B	246	ALA	5.3
1	B	585	ASN	5.2
1	B	218	GLN	4.8
1	A	130	PRO	4.4
1	A	496	TRP	4.3
1	A	292	VAL	4.2
1	A	291	GLY	4.2
1	A	498	GLY	4.1
1	B	104	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	129	ASP	4.1
1	A	584	SER	4.0
1	B	16	LYS	3.9
1	B	219	GLY	3.9
1	B	584	SER	3.8
1	A	245	PRO	3.7
1	A	703	LYS	3.6
1	A	497	ARG	3.5
1	B	131	ALA	3.5
1	B	132	SER	3.5
1	A	127	ASN	3.4
1	B	382	THR	3.4
1	B	127	ASN	3.3
1	A	16	LYS	3.3
1	B	220	GLU	3.3
1	B	245	PRO	2.9
1	A	363	GLY	2.9
1	A	85	GLY	2.9
1	B	243	THR	2.8
1	B	583	ALA	2.8
1	B	362	ALA	2.8
1	B	247	ASP	2.8
1	B	706	ALA	2.7
1	A	359	ASN	2.7
1	B	291	GLY	2.7
1	B	290	ASP	2.6
1	A	83	PRO	2.5
1	B	526	ALA	2.4
1	A	382	THR	2.4
1	B	642	SER	2.3
1	A	585	ASN	2.3
1	A	193	LYS	2.2
1	A	243	THR	2.2
1	B	193	LYS	2.2
1	B	383	ALA	2.2
1	A	681	ARG	2.2
1	B	384	SER	2.2
1	A	455	ASP	2.2
1	A	457	SER	2.2
1	A	456	SER	2.1
1	B	190	SER	2.1
1	B	130	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	17	ILE	2.1
1	B	289	VAL	2.0
1	A	283	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	A	3002	5/5	0.96	0.26	25.01	25,25,31,35	0
2	SO4	A	3001	5/5	0.92	0.14	4.75	19,21,29,49	0
5	GOL	A	902	6/6	0.98	0.05	0.34	12,12,14,19	0
5	GOL	B	1902	6/6	0.99	0.05	-0.14	11,12,14,17	0
4	PHE	B	1904	12/12	0.98	0.05	-0.28	9,10,11,12	0
4	PHE	A	904	12/12	0.98	0.05	-0.46	8,10,11,11	0
3	FAD	B	801	53/53	0.99	0.04	-0.76	8,8,9,13	0
3	FAD	A	801	53/53	0.99	0.04	-1.07	7,8,9,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.