



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:54 AM GMT

PDB ID : 2YR6  
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](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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

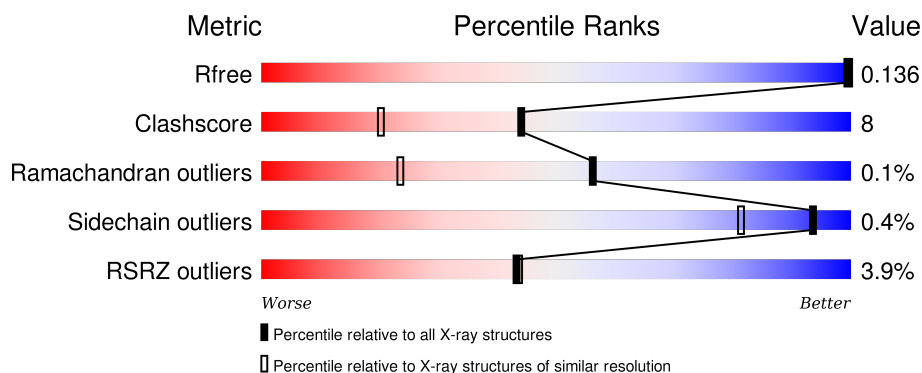
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2199 (1.40-1.32)
Clashscore	102246	2337 (1.40-1.32)
Ramachandran outliers	100387	2280 (1.40-1.32)
Sidechain outliers	100360	2279 (1.40-1.32)
RSRZ outliers	91569	2199 (1.40-1.32)

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	
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	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:

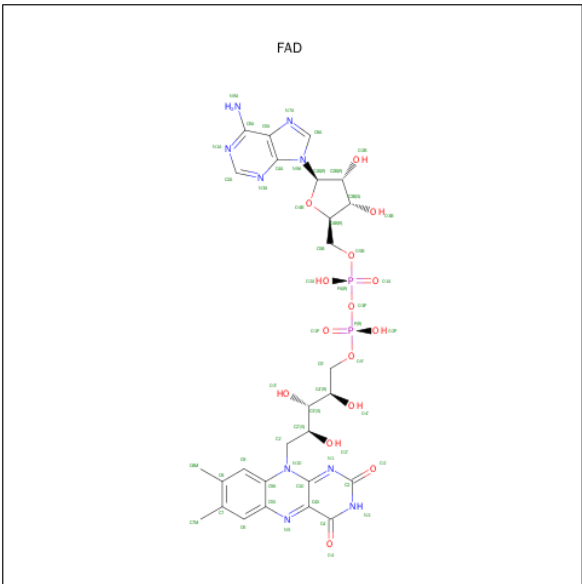
Chain	Residue	Modelled	Actual	Comment	Reference
A	714	LEU	-	EXPRESSION TAG	UNP Q5W9R9
A	715	GLU	-	EXPRESSION TAG	UNP Q5W9R9
A	716	HIS	-	EXPRESSION TAG	UNP Q5W9R9
A	717	HIS	-	EXPRESSION TAG	UNP Q5W9R9
A	718	HIS	-	EXPRESSION TAG	UNP Q5W9R9
A	719	HIS	-	EXPRESSION TAG	UNP Q5W9R9
A	720	HIS	-	EXPRESSION TAG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



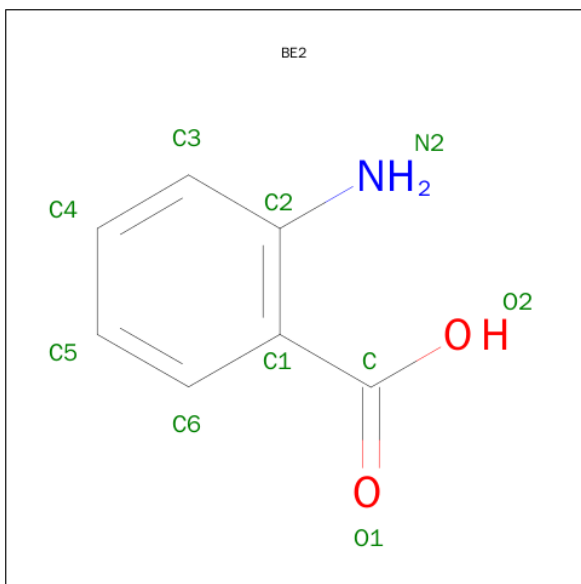
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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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 2-AMINO BENZOIC ACID (three-letter code: 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 (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	1000	Total	O	0	0
			1000	1000		
6	B	957	Total	O	0	0
			957	957		





LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.88Å 113.03Å 136.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.18 – 1.35 34.17 – 1.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.18-1.35) 99.8 (34.17-1.35)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.51 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.103 , 0.138 0.105 , 0.136	Depositor DCC
$R_{free}$ test set	17132 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	11.7	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 58.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 339203 reflections	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	12529	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: BE2, 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	1.54	68/5347 (1.3%)	1.51	74/7300 (1.0%)
1	B	1.49	58/5347 (1.1%)	1.43	69/7300 (0.9%)
All	All	1.52	126/10694 (1.2%)	1.47	143/14600 (1.0%)

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 (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	297	GLU	CD-OE2	21.49	1.49	1.25
1	A	576	ARG	CZ-NH1	17.53	1.55	1.33
1	A	245	PRO	N-CA	16.90	1.75	1.47
1	A	246	ALA	C-O	15.06	1.51	1.23
1	A	323	SER	CB-OG	-14.52	1.23	1.42
1	B	576	ARG	CZ-NH2	13.87	1.51	1.33
1	B	224	MET	CB-CG	13.80	1.95	1.51
1	A	323	SER	CA-CB	12.46	1.71	1.52
1	A	642	SER	CB-OG	11.51	1.57	1.42
1	B	58	ARG	CZ-NH2	11.14	1.47	1.33
1	A	245	PRO	CB-CG	10.45	2.02	1.50
1	B	544	ARG	CD-NE	10.21	1.63	1.46
1	A	576	ARG	CD-NE	-10.08	1.29	1.46
1	A	147	ILE	CB-CG1	-9.72	1.26	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	544	ARG	NE-CZ	-9.69	1.20	1.33
1	B	642	SER	CB-OG	9.38	1.54	1.42
1	B	323	SER	CB-OG	-9.34	1.30	1.42
1	A	576	ARG	NE-CZ	9.19	1.45	1.33
1	A	422	SER	CA-CB	8.99	1.66	1.52
1	A	544	ARG	CD-NE	8.97	1.61	1.46
1	A	77	ARG	CZ-NH2	-8.84	1.21	1.33
1	B	297	GLU	CG-CD	8.67	1.65	1.51
1	B	546	ARG	CZ-NH2	-8.62	1.21	1.33
1	B	544	ARG	CZ-NH2	-8.51	1.22	1.33
1	B	642	SER	CA-CB	8.37	1.65	1.52
1	B	296	ASP	CB-CG	-8.32	1.34	1.51
1	A	684	VAL	CB-CG2	-8.31	1.35	1.52
1	A	282	GLU	CD-OE2	8.29	1.34	1.25
1	A	245	PRO	CA-C	8.29	1.69	1.52
1	A	245	PRO	C-O	8.22	1.39	1.23
1	A	147	ILE	CB-CG2	8.03	1.77	1.52
1	B	386	ARG	CB-CG	-7.89	1.31	1.52
1	A	690	GLU	CD-OE1	7.81	1.34	1.25
1	B	364	LYS	CE-NZ	-7.79	1.29	1.49
1	A	456	SER	CB-OG	7.72	1.52	1.42
1	B	546	ARG	CZ-NH1	-7.72	1.23	1.33
1	A	246	ALA	CA-CB	-7.65	1.36	1.52
1	A	568	ARG	CG-CD	-7.56	1.33	1.51
1	B	282	GLU	CD-OE2	7.44	1.33	1.25
1	A	544	ARG	CZ-NH2	-7.43	1.23	1.33
1	A	282	GLU	CG-CD	7.37	1.63	1.51
1	B	568	ARG	CD-NE	-7.30	1.34	1.46
1	A	546	ARG	CG-CD	7.27	1.70	1.51
1	A	706	ALA	CA-CB	7.27	1.67	1.52
1	B	544	ARG	CG-CD	7.26	1.70	1.51
1	B	692	ARG	CZ-NH2	-7.21	1.23	1.33
1	B	544	ARG	NE-CZ	-7.21	1.23	1.33
1	B	147	ILE	CB-CG2	7.18	1.75	1.52
1	A	576	ARG	CZ-NH2	-7.15	1.23	1.33
1	A	463	ARG	CB-CG	-7.07	1.33	1.52
1	B	292	VAL	N-CA	7.05	1.60	1.46
1	A	338	GLU	CD-OE2	7.04	1.33	1.25
1	B	370	ARG	CZ-NH2	-6.95	1.24	1.33
1	B	339	TYR	CE2-CZ	-6.85	1.29	1.38
1	B	204	LYS	CD-CE	6.83	1.68	1.51
1	B	301	TYR	CG-CD2	-6.83	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	SER	CB-OG	-6.80	1.33	1.42
1	B	425	GLU	CG-CD	6.80	1.62	1.51
1	A	290	ASP	CB-CG	6.79	1.66	1.51
1	A	23	GLU	CD-OE1	-6.75	1.18	1.25
1	A	579	LYS	CD-CE	6.51	1.67	1.51
1	B	301	TYR	CE2-CZ	-6.46	1.30	1.38
1	A	692	ARG	CZ-NH2	-6.43	1.24	1.33
1	B	283	LYS	CB-CG	-6.43	1.35	1.52
1	A	362	ALA	CA-CB	6.42	1.66	1.52
1	A	599	ARG	NE-CZ	6.39	1.41	1.33
1	B	684	VAL	CB-CG2	-6.37	1.39	1.52
1	A	250	GLU	CG-CD	-6.28	1.42	1.51
1	A	196	GLU	CD-OE1	6.28	1.32	1.25
1	A	220	GLU	CB-CG	-6.28	1.40	1.52
1	A	146	GLU	CD-OE1	-6.22	1.18	1.25
1	B	32	ARG	CG-CD	-6.20	1.36	1.51
1	B	58	ARG	CZ-NH1	6.14	1.41	1.33
1	A	204	LYS	CB-CG	-6.14	1.35	1.52
1	B	204	LYS	CE-NZ	-6.10	1.33	1.49
1	A	463	ARG	CG-CD	6.08	1.67	1.51
1	B	609	THR	CB-CG2	-6.04	1.32	1.52
1	A	455	ASP	CB-CG	6.00	1.64	1.51
1	A	345	GLU	CG-CD	-5.90	1.43	1.51
1	A	246	ALA	C-N	5.87	1.47	1.34
1	B	193	LYS	CE-NZ	5.87	1.63	1.49
1	B	338	GLU	CD-OE2	5.87	1.32	1.25
1	A	568	ARG	NE-CZ	5.82	1.40	1.33
1	B	190	SER	CA-CB	5.82	1.61	1.52
1	A	27	SER	CB-OG	-5.81	1.34	1.42
1	B	577	TYR	CD1-CE1	-5.80	1.30	1.39
1	A	244	PRO	C-N	-5.79	1.23	1.34
1	A	32	ARG	CG-CD	-5.79	1.37	1.51
1	A	425	GLU	CD-OE1	-5.78	1.19	1.25
1	B	364	LYS	CG-CD	-5.77	1.32	1.52
1	B	259	GLU	CD-OE1	5.74	1.31	1.25
1	A	568	ARG	CD-NE	-5.74	1.36	1.46
1	A	502	LYS	CG-CD	5.71	1.71	1.52
1	A	77	ARG	CD-NE	-5.68	1.36	1.46
1	B	147	ILE	CB-CG1	-5.63	1.38	1.54
1	B	425	GLU	CD-OE2	-5.63	1.19	1.25
1	B	422	SER	CA-CB	5.51	1.61	1.52
1	A	428	ALA	CA-CB	5.50	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	597	GLU	CD-OE1	-5.50	1.19	1.25
1	B	77	ARG	CD-NE	-5.47	1.37	1.46
1	B	384	SER	CA-CB	5.41	1.61	1.52
1	B	292	VAL	CB-CG2	5.39	1.64	1.52
1	A	588	PRO	N-CD	5.38	1.55	1.47
1	B	360	VAL	CB-CG2	-5.33	1.41	1.52
1	A	702	VAL	CB-CG1	5.25	1.63	1.52
1	B	425	GLU	CB-CG	-5.24	1.42	1.52
1	A	592	TYR	CG-CD2	-5.24	1.32	1.39
1	A	580	TYR	CE2-CZ	-5.24	1.31	1.38
1	A	16	LYS	CD-CE	5.24	1.64	1.51
1	B	643	LEU	C-N	-5.24	1.22	1.34
1	A	77	ARG	CZ-NH1	5.22	1.39	1.33
1	B	190	SER	CB-OG	5.17	1.49	1.42
1	B	51	ARG	CG-CD	5.16	1.64	1.51
1	A	380	SER	CB-OG	-5.15	1.35	1.42
1	B	559	GLU	CD-OE1	-5.15	1.20	1.25
1	B	690	GLU	CG-CD	5.13	1.59	1.51
1	A	627	GLN	CG-CD	-5.11	1.39	1.51
1	A	690	GLU	CB-CG	-5.10	1.42	1.52
1	B	702	VAL	CB-CG2	5.09	1.63	1.52
1	A	559	GLU	CG-CD	5.08	1.59	1.51
1	A	263	GLN	CB-CG	-5.07	1.38	1.52
1	B	429	SER	CB-OG	-5.05	1.35	1.42
1	A	147	ILE	CA-CB	-5.04	1.43	1.54
1	B	196	GLU	CG-CD	-5.04	1.44	1.51
1	B	301	TYR	CB-CG	5.04	1.59	1.51
1	A	128	GLY	N-CA	5.03	1.53	1.46

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	576	ARG	NE-CZ-NH1	30.50	135.55	120.30
1	B	576	ARG	NE-CZ-NH1	-23.09	108.76	120.30
1	B	576	ARG	NE-CZ-NH2	22.44	131.52	120.30
1	A	576	ARG	NE-CZ-NH2	-21.99	109.31	120.30
1	A	646	ARG	NE-CZ-NH2	-21.09	109.76	120.30
1	B	568	ARG	NE-CZ-NH1	20.48	130.54	120.30
1	A	599	ARG	NE-CZ-NH1	20.38	130.49	120.30
1	A	546	ARG	NE-CZ-NH1	18.94	129.77	120.30
1	A	646	ARG	NE-CZ-NH1	18.52	129.56	120.30
1	B	546	ARG	NE-CZ-NH1	16.64	128.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	599	ARG	NE-CZ-NH2	-14.51	113.04	120.30
1	A	77	ARG	NE-CZ-NH1	14.48	127.54	120.30
1	B	224	MET	CG-SD-CE	-14.13	77.59	100.20
1	A	544	ARG	NE-CZ-NH2	13.92	127.26	120.30
1	B	599	ARG	NE-CZ-NH1	13.16	126.88	120.30
1	A	370	ARG	NE-CZ-NH2	-12.99	113.81	120.30
1	B	699	ARG	NE-CZ-NH2	-12.10	114.25	120.30
1	B	692	ARG	NE-CZ-NH1	12.01	126.30	120.30
1	B	296	ASP	CB-CG-OD2	-11.36	108.08	118.30
1	A	77	ARG	NE-CZ-NH2	-11.35	114.62	120.30
1	B	568	ARG	NE-CZ-NH2	-11.31	114.64	120.30
1	A	568	ARG	NE-CZ-NH2	10.27	125.43	120.30
1	A	370	ARG	NE-CZ-NH1	10.19	125.40	120.30
1	A	455	ASP	CB-CG-OD2	10.17	127.46	118.30
1	A	294	ASP	CB-CG-OD1	9.82	127.14	118.30
1	B	290	ASP	CB-CG-OD2	-9.74	109.53	118.30
1	A	546	ARG	NH1-CZ-NH2	-9.57	108.87	119.40
1	A	293	LEU	CB-CG-CD1	9.57	127.27	111.00
1	B	599	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	B	256	TYR	CD1-CE1-CZ	-9.33	111.40	119.80
1	B	607	ASP	CB-CG-OD2	-9.00	110.20	118.30
1	A	245	PRO	O-C-N	-8.97	108.35	122.70
1	B	386	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	B	274	ARG	NE-CZ-NH1	8.59	124.60	120.30
1	B	274	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	B	89	ASP	CB-CG-OD1	8.31	125.78	118.30
1	B	77	ARG	CD-NE-CZ	8.30	135.22	123.60
1	B	256	TYR	CZ-CE2-CD2	-8.19	112.43	119.80
1	A	546	ARG	CD-NE-CZ	8.14	135.00	123.60
1	A	246	ALA	O-C-N	8.04	135.56	122.70
1	B	544	ARG	NE-CZ-NH2	7.99	124.29	120.30
1	A	245	PRO	CA-N-CD	7.97	122.86	111.70
1	A	245	PRO	N-CA-C	7.96	132.81	112.10
1	B	370	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	B	203	LEU	CB-CG-CD1	7.87	124.38	111.00
1	A	603	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	B	199	ASP	CB-CG-OD1	-7.80	111.28	118.30
1	B	421	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	247	ASP	CB-CG-OD1	-7.74	111.34	118.30
1	B	297	GLU	CG-CD-OE1	-7.73	102.83	118.30
1	A	576	ARG	CG-CD-NE	-7.71	95.61	111.80
1	B	497	ARG	NE-CZ-NH1	7.70	124.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	692	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	A	692	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	B	203	LEU	CB-CG-CD2	-7.60	98.09	111.00
1	A	89	ASP	CB-CG-OD1	7.49	125.04	118.30
1	A	576	ARG	CD-NE-CZ	-7.40	113.23	123.60
1	A	626	HIS	CG-ND1-CE1	-7.35	96.15	105.70
1	B	256	TYR	CE1-CZ-CE2	7.30	131.48	119.80
1	B	564	ASP	CB-CG-OD1	7.26	124.83	118.30
1	B	77	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	A	475	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	701	VAL	CG1-CB-CG2	7.08	122.23	110.90
1	A	633	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	B	364	LYS	CD-CE-NZ	-7.05	95.48	111.70
1	A	546	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	B	644	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	A	364	LYS	CD-CE-NZ	-6.90	95.83	111.70
1	A	699	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	A	244	PRO	C-N-CA	-6.80	93.45	122.00
1	A	353	LEU	CB-CG-CD2	-6.74	99.55	111.00
1	A	463	ARG	CG-CD-NE	-6.73	97.67	111.80
1	B	690	GLU	OE1-CD-OE2	-6.71	115.25	123.30
1	A	568	ARG	NH1-CZ-NH2	-6.64	112.09	119.40
1	B	370	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	A	244	PRO	C-N-CD	6.60	142.27	128.40
1	A	245	PRO	CA-C-O	6.53	135.87	120.20
1	B	251	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	A	205	VAL	CA-CB-CG1	6.33	120.39	110.90
1	B	539	GLU	OE1-CD-OE2	-6.19	115.87	123.30
1	A	587	GLN	N-CA-CB	-6.16	99.52	110.60
1	B	308	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	B	576	ARG	CD-NE-CZ	6.13	132.18	123.60
1	A	275	GLU	OE1-CD-OE2	6.12	130.65	123.30
1	B	568	ARG	CD-NE-CZ	6.12	132.17	123.60
1	B	643	LEU	O-C-N	-6.06	113.00	122.70
1	A	386	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	A	607	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	A	103	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	B	297	GLU	CG-CD-OE2	5.88	130.07	118.30
1	B	113	ARG	NE-CZ-NH2	5.87	123.23	120.30
1	A	146	GLU	OE1-CD-OE2	-5.85	116.28	123.30
1	B	405	PHE	CB-CG-CD1	5.82	124.87	120.80
1	A	692	ARG	NE-CZ-NH1	5.81	123.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	TYR	CB-CG-CD1	5.71	124.43	121.00
1	A	349	PHE	CB-CG-CD2	-5.71	116.81	120.80
1	A	247	ASP	CB-CA-C	5.69	121.79	110.40
1	B	137	TYR	CB-CG-CD2	5.64	124.39	121.00
1	A	373	ARG	CD-NE-CZ	5.61	131.45	123.60
1	A	301	TYR	CB-CG-CD2	5.60	124.36	121.00
1	A	544	ARG	NH1-CZ-NH2	-5.59	113.26	119.40
1	A	320	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	B	58	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	B	292	VAL	CA-CB-CG1	5.54	119.21	110.90
1	B	143	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	338	GLU	OE1-CD-OE2	-5.52	116.67	123.30
1	A	463	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	455	ASP	CB-CA-C	-5.51	99.39	110.40
1	B	633	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	247	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	302	TYR	CD1-CE1-CZ	-5.47	114.88	119.80
1	B	302	TYR	CB-CG-CD1	-5.45	117.73	121.00
1	B	546	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	93	TYR	CD1-CE1-CZ	-5.40	114.94	119.80
1	B	643	LEU	C-N-CA	-5.38	108.25	121.70
1	B	544	ARG	CG-CD-NE	5.37	123.08	111.80
1	A	292	VAL	CA-CB-CG2	-5.37	102.84	110.90
1	A	597	GLU	OE1-CD-OE2	5.33	129.70	123.30
1	B	203	LEU	CD1-CG-CD2	5.33	126.49	110.50
1	A	392	TYR	CB-CG-CD2	5.33	124.20	121.00
1	A	349	PHE	CB-CG-CD1	5.32	124.52	120.80
1	B	224	MET	CB-CG-SD	-5.31	96.47	112.40
1	B	699	ARG	NH1-CZ-NH2	5.26	125.19	119.40
1	B	58	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	B	646	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	A	166	LYS	CD-CE-NZ	5.22	123.71	111.70
1	B	690	GLU	CG-CD-OE1	5.21	128.72	118.30
1	A	702	VAL	N-CA-C	-5.21	96.94	111.00
1	A	247	ASP	N-CA-CB	5.21	119.97	110.60
1	A	30	ASN	CB-CG-OD1	-5.20	111.20	121.60
1	B	191	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	143	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	A	373	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	463	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	B	301	TYR	CG-CD2-CE2	5.12	125.40	121.30
1	B	316	PHE	CB-CG-CD1	5.11	124.38	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	ARG	CA-CB-CG	-5.10	102.18	113.40
1	B	546	ARG	NH1-CZ-NH2	-5.10	113.79	119.40
1	A	316	PHE	CB-CG-CD2	-5.09	117.24	120.80
1	A	373	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	A	678	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	246	ALA	C-N-CA	-5.01	109.18	121.70
1	A	393	ASP	CB-CG-OD2	-5.00	113.80	118.30

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
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	102	1
1	B	5212	0	5102	68	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	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	10	0	6	0	0
5	A	6	0	7	0	0
5	B	6	0	8	0	0
6	A	1000	0	0	63	8
6	B	957	0	0	41	7
All	All	12529	0	10293	167	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 (167) 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:CA	1:A:245:PRO:N	1.76	1.47
1:B:224:MET:CB	1:B:224:MET:CG	1.95	1.43
1:A:245:PRO:CG	1:A:245:PRO:CB	2.02	1.38
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:B:224:MET:CE	6:B:3930:HOH:O	1.85	1.24
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: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:224:MET:HE3	6:B:3930:HOH:O	1.43	1.12
1:A:244:PRO:C	1:A:245:PRO:CA	2.20	1.10
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: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:CG1	1:A:147:ILE:CG2	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:A:244:PRO:O	1:A:245:PRO:HA	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:224:MET:SD	1:B:224:MET:CB	2.72	0.76
1:A:113:ARG:HD3	6:A:3980:HOH:O	1.85	0.76
1:A:422:SER:HB3	6:A:3433:HOH:O	1.86	0.75
1:B:147:ILE:CA	1:B:147:ILE:CG2	2.65	0.74
1:B:224:MET:HE2	6:B:3930:HOH:O	1.63	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:CG1	1:B:147:ILE:CG2	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: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:224:MET:HE3	6:A:3559:HOH:O	1.93	0.67
1:A:246:ALA:CB	6:A:3430:HOH:O	2.35	0.67
1:A:292:VAL:CG2	1:A:292:VAL:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:626:HIS:CE1	6:A:3248:HOH:O	2.48	0.63
1:A:204:LYS:CE	6:A:3908:HOH:O	2.46	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
1:A:218:GLN:CD	6:A:3951:HOH:O	2.35	0.61
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:224:MET:CE	6:A:3559:HOH:O	2.47	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:A:245:PRO:O	1:A:246:ALA:C	2.41	0.58
1:B:475:ARG:HG2	2:B:3001:SO4:O4	2.04	0.57
1:B:412:HIS:HD2	1:B:653:SER:OG	1.87	0.57
1:B:153:HIS:HE1	6:B:3118:HOH:O	1.87	0.57
1:B:89:ASP:OD2	6:B:3928:HOH:O	2.17	0.57
1:B:147:ILE:HB	1:B:147:ILE:CG2	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:B:379:HIS:CE1	1:B:646:ARG:H	2.15	0.56
6:A:3976:HOH:O	1:B:293:LEU:CD2	2.50	0.56
1:A:455:ASP:HA	6:A:3934:HOH:O	2.06	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:361:GLY:C	6:A:3425:HOH:O	2.49	0.51
1:A:446:GLN:NE2	6:A:3472:HOH:O	2.30	0.51
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
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: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:A:204:LYS:HG3	6:A:3675:HOH:O	2.14	0.47
1:A:626:HIS:CE1	6:A:3337:HOH:O	2.67	0.46
1:A:463:ARG:HG2	6:B:3912:HOH:O	2.15	0.46
1:A:245:PRO:CG	1:A:245:PRO:CA	2.72	0.46
1:A:127:ASN:CB	6:A:3956:HOH:O	2.20	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:546:ARG:NH2	1:A:609:THR:OG1	2.49	0.46
1:A:83:PRO:HD3	6:A:3703:HOH:O	2.16	0.46
1:A:104:ARG:C	6:A:3966:HOH:O	2.55	0.46
1:A:559:GLU:CD	6:A:3893:HOH:O	2.52	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CA	1:A:147:ILE:CG2	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: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
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:3472:HOH:O	6:B:3826:HOH:O[2_665]	2.19	0.01
6:A:3440:HOH:O	6:A:3814:HOH:O[3_756]	2.19	0.01

## 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%)	663 (98%)	15 (2%)	0	100	100
1	B	678/721 (94%)	662 (98%)	15 (2%)	1 (0%)	56	23
All	All	1356/1442 (94%)	1325 (98%)	30 (2%)	1 (0%)	56	23

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%)	532 (100%)	2 (0%)	93	81
1	B	534/566 (94%)	532 (100%)	2 (0%)	93	81
All	All	1068/1132 (94%)	1064 (100%)	4 (0%)	93	81

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ARG
1	A	247	ASP
1	B	292	VAL
1	B	294	ASP

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

Mol	Chain	Res	Type
1	A	127	ASN
1	A	216	ASN
1	A	395	HIS
1	A	399	HIS

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Mol	Chain	Res	Type
1	A	412	HIS
1	A	472	HIS
1	A	495	GLN
1	A	547	HIS
1	A	587	GLN
1	A	626	HIS
1	B	102	HIS
1	B	153	HIS
1	B	379	HIS
1	B	399	HIS
1	B	412	HIS
1	B	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	3002	-	4,4,4	1.81	1 (25%)	6,6,6	3.18	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FAD	A	801	-	48,58,58	1.68	8 (16%)	54,89,89	2.12	6 (11%)
5	GOL	A	902	-	5,5,5	1.30	0	5,5,5	0.90	0
4	BE2	A	906	-	7,10,10	1.11	1 (14%)	8,13,13	2.41	3 (37%)
5	GOL	B	1902	-	5,5,5	0.50	0	5,5,5	0.63	0
4	BE2	B	1906	-	7,10,10	1.74	1 (14%)	8,13,13	1.96	2 (25%)
2	SO4	B	3001	-	4,4,4	2.25	2 (50%)	6,6,6	2.30	3 (50%)
3	FAD	B	801	-	48,58,58	1.34	6 (12%)	54,89,89	2.39	14 (25%)

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	3002	-	-	0/0/0/0	0/0/0/0
3	FAD	A	801	-	-	0/30/50/50	0/6/6/6
5	GOL	A	902	-	-	0/4/4/4	0/0/0/0
4	BE2	A	906	-	-	0/0/4/4	0/1/1/1
5	GOL	B	1902	-	-	0/4/4/4	0/0/0/0
4	BE2	B	1906	-	-	0/0/4/4	0/1/1/1
2	SO4	B	3001	-	-	0/0/0/0	0/0/0/0
3	FAD	B	801	-	-	0/30/50/50	0/6/6/6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	FAD	C10-N10	-4.58	1.33	1.39
3	B	801	FAD	C1'-N10	-4.56	1.43	1.48
2	B	3001	SO4	O2-S	-2.88	1.37	1.47
2	B	3001	SO4	O1-S	-2.49	1.38	1.47
3	A	801	FAD	C9-C9A	-2.42	1.35	1.40
3	B	801	FAD	C6-C5X	-2.31	1.38	1.41
3	B	801	FAD	C4X-N5	2.25	1.36	1.33
3	A	801	FAD	C5B-C4B	2.25	1.58	1.51
3	B	801	FAD	O2'-C2'	2.29	1.48	1.43
4	A	906	BE2	C5-C6	2.34	1.43	1.38
3	A	801	FAD	C2A-N1A	2.38	1.38	1.33
3	A	801	FAD	C4-N3	2.47	1.37	1.33
3	B	801	FAD	C4-N3	2.77	1.38	1.33
2	A	3002	SO4	O4-S	3.14	1.58	1.47
3	A	801	FAD	C4X-N5	3.34	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	FAD	O4B-C1B	3.47	1.45	1.41
4	B	1906	BE2	C1-C2	4.03	1.47	1.41
3	A	801	FAD	C9A-N10	4.50	1.45	1.38
3	A	801	FAD	O4B-C1B	5.47	1.48	1.41

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	FAD	C4-C4X-C10	-7.62	115.07	119.94
3	A	801	FAD	C4X-C4-N3	-5.93	115.48	123.59
3	B	801	FAD	C4X-C10-N10	-5.58	117.23	120.52
4	A	906	BE2	C4-C5-C6	-3.75	114.69	120.19
3	B	801	FAD	C4X-C4-N3	-3.41	118.92	123.59
3	A	801	FAD	C9A-C5X-N5	-3.34	117.41	122.36
2	B	3001	SO4	O4-S-O3	-3.05	96.56	108.98
3	B	801	FAD	C9A-C5X-N5	-2.95	117.99	122.36
2	B	3001	SO4	O4-S-O2	-2.76	84.54	110.19
4	B	1906	BE2	C4-C5-C6	-2.66	116.29	120.19
3	A	801	FAD	C4B-O4B-C1B	-2.50	106.98	109.72
3	B	801	FAD	C1B-N9A-C4A	-2.14	123.72	126.94
3	B	801	FAD	C6-C7-C8	-2.12	115.99	120.04
3	B	801	FAD	O4B-C4B-C3B	2.27	109.73	105.15
3	A	801	FAD	C4-C4X-N5	2.32	121.54	118.72
3	B	801	FAD	C6-C5X-N5	2.67	122.39	118.96
3	B	801	FAD	C7-C6-C5X	2.80	125.49	120.92
4	A	906	BE2	C5-C6-C1	2.80	125.20	120.33
2	A	3002	SO4	O4-S-O3	3.07	121.47	108.98
2	B	3001	SO4	O2-S-O1	3.27	119.84	109.50
3	B	801	FAD	C5X-C9A-N10	3.53	120.30	117.62
3	B	801	FAD	C4X-N5-C5X	3.54	120.84	116.76
3	B	801	FAD	C4-C4X-N5	4.03	123.61	118.72
3	B	801	FAD	C1'-N10-C9A	4.16	123.53	118.86
4	A	906	BE2	C3-C2-C1	4.30	122.50	118.10
4	B	1906	BE2	C5-C6-C1	4.44	128.06	120.33
3	A	801	FAD	C4X-N5-C5X	5.32	122.88	116.76
2	A	3002	SO4	O2-S-O1	6.79	131.03	109.50
3	B	801	FAD	C4-N3-C2	8.82	122.87	115.25
3	A	801	FAD	C4-N3-C2	10.33	124.17	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

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

## 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, 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%)	-0.20	29 (4%) 40 40	8, 14, 28, 47	0
1	B	684/721 (94%)	-0.23	25 (3%) 45 46	9, 14, 29, 42	0
All	All	1368/1442 (94%)	-0.21	54 (3%) 43 44	8, 14, 29, 47	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	707	ALA	11.6
1	B	707	ALA	8.1
1	A	104	ARG	7.4
1	A	246	ALA	6.4
1	A	362	ALA	6.3
1	B	521	VAL	6.3
1	B	292	VAL	6.3
1	A	706	ALA	6.1
1	A	521	VAL	6.0
1	A	496	TRP	5.1
1	B	246	ALA	5.0
1	A	131	ALA	4.8
1	A	132	SER	4.7
1	B	293	LEU	4.5
1	A	705	PRO	4.4
1	B	104	ARG	4.3
1	A	497	ARG	4.3
1	A	704	VAL	4.2
1	B	382	THR	3.9
1	B	585	ASN	3.7
1	B	243	THR	3.6
1	B	526	ALA	3.5
1	B	218	GLN	3.5
1	A	292	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	703	LYS	3.3
1	B	706	ALA	3.3
1	A	130	PRO	3.3
1	A	128	GLY	3.2
1	A	498	GLY	3.2
1	A	245	PRO	3.2
1	B	16	LYS	3.1
1	B	584	SER	3.0
1	A	193	LYS	3.0
1	A	16	LYS	3.0
1	B	131	ALA	3.0
1	A	85	GLY	2.9
1	B	705	PRO	2.9
1	B	132	SER	2.9
1	A	584	SER	2.9
1	A	129	ASP	2.8
1	A	291	GLY	2.8
1	B	220	GLU	2.6
1	A	526	ALA	2.6
1	B	362	ALA	2.5
1	B	219	GLY	2.5
1	A	382	THR	2.5
1	B	290	ASP	2.4
1	B	383	ALA	2.4
1	B	17	ILE	2.3
1	B	291	GLY	2.2
1	A	127	ASN	2.2
1	A	283	LYS	2.2
1	B	127	ASN	2.1
1	A	363	GLY	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	0.98	0.16	12.79	32,36,37,43	0
2	SO4	B	3001	5/5	0.97	0.17	11.25	30,32,33,47	0
5	GOL	B	1902	6/6	0.97	0.06	1.44	14,15,18,21	0
4	BE2	A	906	10/10	0.95	0.07	0.64	12,14,16,16	0
4	BE2	B	1906	10/10	0.96	0.06	-0.14	13,14,16,16	0
3	FAD	B	801	53/53	0.99	0.05	-0.62	8,9,10,11	0
3	FAD	A	801	53/53	0.99	0.06	-0.86	7,9,10,10	0
5	GOL	A	902	6/6	0.98	0.04	-1.21	15,16,20,26	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.