



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:46 PM GMT

PDB ID : 1QLU  
Title : STRUCTURE OF THE H422A MUTANT VANILLYL-ALCOHOL OXIDASE  
IN COMPLEX WITH ISOEUGENOL  
Authors : Mattevi, A.  
Deposited on : 1999-09-16  
Resolution : 2.40 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

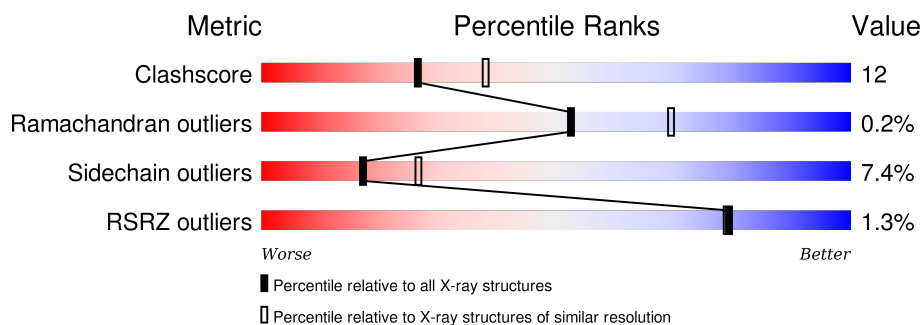
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	560	
1	B	560	

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
3	EUG	B	601	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9076 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.

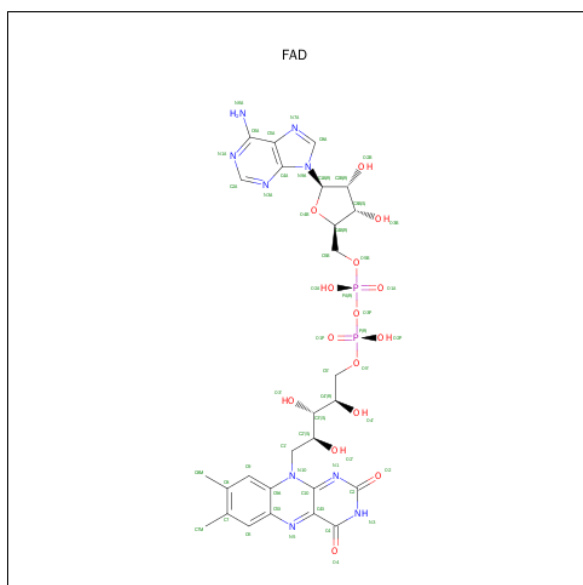
- Molecule 1 is a protein called VANILLYL-ALCOHOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	66	0	0
			4346	2790	742	790	24			
1	B	550	Total	C	N	O	S	66	0	0
			4346	2790	742	790	24			

There are 4 discrepancies between the modelled and reference sequences:

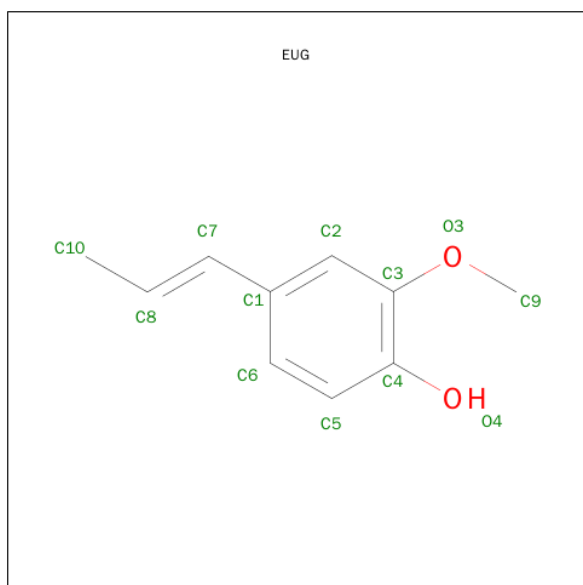
Chain	Residue	Modelled	Actual	Comment	Reference
A	274	GLY	ARG	CONFLICT	UNP P56216
A	422	ALA	HIS	ENGINEERED MUTATION	UNP P56216
B	274	GLY	ARG	CONFLICT	UNP P56216
B	422	ALA	HIS	ENGINEERED MUTATION	UNP P56216

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

- Molecule 3 is 2-METHOXY-4-[(1E)-PROP-1-EN-1-YL]PHENOL (three-letter code: EUG) (formula: C<sub>10</sub>H<sub>12</sub>O<sub>2</sub>).



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

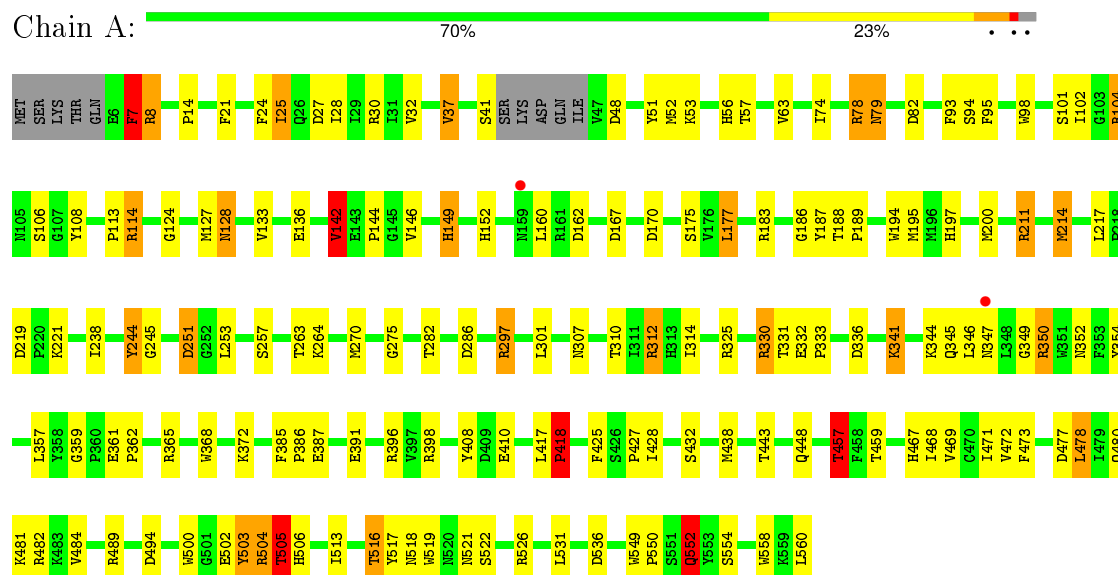
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	139	Total	O	0	0
			139	139		
4	B	117	Total	O	0	0
			117	117		

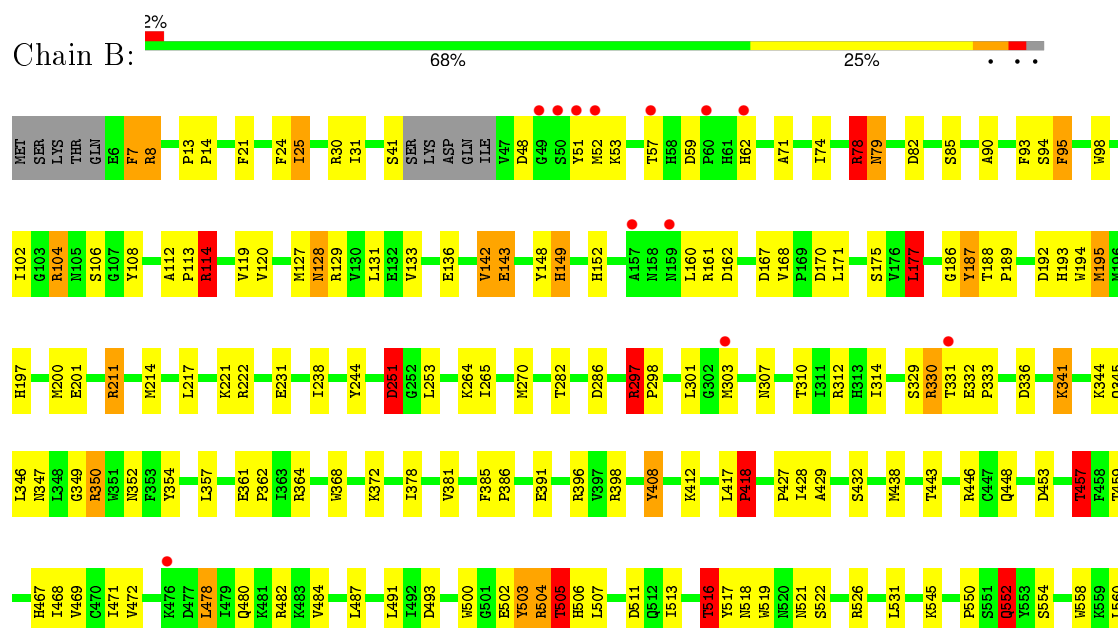
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: VANILLYL-ALCOHOL OXIDASE



#### • Molecule 1: VANILLYL-ALCOHOL OXIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.84Å 129.84Å 133.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 34.78 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.8 (30.00-2.40) 91.4 (34.78-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.219 , 0.273 0.212 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.1	EDS
Estimated twinning fraction	0.006 for l,-k,h 0.023 for -l,-k,-h 0.022 for -h,-l,-k 0.006 for -h,l,k 0.040 for -h,k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 51342 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9076	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: EUG, 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	0.85	4/4464 (0.1%)	1.81	70/6067 (1.2%)
1	B	0.87	3/4464 (0.1%)	1.82	74/6067 (1.2%)
All	All	0.86	7/8928 (0.1%)	1.81	144/12134 (1.2%)

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	1
1	B	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	52	MET	CB-CG	32.54	2.55	1.51
1	A	52	MET	CB-CG	31.09	2.50	1.51
1	B	350	ARG	CZ-NH1	11.33	1.47	1.33
1	A	350	ARG	CZ-NH1	11.02	1.47	1.33
1	B	372	LYS	CD-CE	-7.34	1.32	1.51
1	A	372	LYS	CD-CE	-5.97	1.36	1.51
1	A	341	LYS	CB-CG	-5.21	1.38	1.52

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	350	ARG	NE-CZ-NH1	-57.46	91.57	120.30
1	A	350	ARG	NE-CZ-NH1	-57.14	91.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	ARG	CA-CB-CG	22.37	162.62	113.40
1	B	211	ARG	CD-NE-CZ	21.41	153.58	123.60
1	A	211	ARG	CD-NE-CZ	19.97	151.56	123.60
1	A	52	MET	CA-CB-CG	-17.53	83.50	113.30
1	A	114	ARG	NE-CZ-NH2	-17.00	111.80	120.30
1	A	211	ARG	CA-CB-CG	16.57	149.87	113.40
1	B	52	MET	CA-CB-CG	-16.51	85.23	113.30
1	A	350	ARG	NE-CZ-NH2	16.10	128.35	120.30
1	B	350	ARG	NE-CZ-NH2	14.56	127.58	120.30
1	B	504	ARG	NE-CZ-NH2	-14.26	113.17	120.30
1	A	504	ARG	NE-CZ-NH2	-13.22	113.69	120.30
1	A	297	ARG	NE-CZ-NH2	-13.08	113.76	120.30
1	B	114	ARG	NE-CZ-NH1	12.50	126.55	120.30
1	B	170	ASP	CB-CG-OD1	12.37	129.43	118.30
1	B	297	ARG	CD-NE-CZ	12.20	140.68	123.60
1	B	446	ARG	NE-CZ-NH1	12.09	126.34	120.30
1	B	114	ARG	NE-CZ-NH2	-11.66	114.47	120.30
1	A	297	ARG	CD-NE-CZ	11.49	139.69	123.60
1	A	114	ARG	CB-CG-CD	11.27	140.90	111.60
1	A	482	ARG	NE-CZ-NH1	11.21	125.91	120.30
1	A	114	ARG	NE-CZ-NH1	11.18	125.89	120.30
1	B	482	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	A	297	ARG	NE-CZ-NH1	11.11	125.86	120.30
1	B	482	ARG	NE-CZ-NH1	11.05	125.83	120.30
1	A	251	ASP	CB-CG-OD1	10.33	127.59	118.30
1	A	330	ARG	NE-CZ-NH2	9.97	125.29	120.30
1	A	30	ARG	CA-CB-CG	9.64	134.61	113.40
1	A	552	GLN	CA-CB-CG	9.47	134.24	113.40
1	B	211	ARG	NE-CZ-NH1	-9.41	115.59	120.30
1	A	489	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	B	211	ARG	NE-CZ-NH2	9.33	124.96	120.30
1	B	30	ARG	CA-CB-CG	9.30	133.85	113.40
1	A	341	LYS	CA-CB-CG	9.19	133.61	113.40
1	B	251	ASP	CB-CG-OD1	9.09	126.48	118.30
1	A	214	MET	CG-SD-CE	9.09	114.74	100.20
1	B	552	GLN	CA-CB-CG	8.47	132.03	113.40
1	A	104	ARG	CD-NE-CZ	8.46	135.45	123.60
1	B	398	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	A	536	ASP	CB-CG-OD1	8.35	125.81	118.30
1	A	128	ASN	CB-CA-C	-8.31	93.78	110.40
1	B	104	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	A	183	ARG	NE-CZ-NH1	-8.25	116.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ASP	CB-CG-OD2	8.12	125.61	118.30
1	A	526	ARG	CD-NE-CZ	8.11	134.95	123.60
1	B	482	ARG	CD-NE-CZ	8.10	134.94	123.60
1	B	398	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	B	297	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	A	221	LYS	CB-CG-CD	7.91	132.18	111.60
1	A	8	ARG	NE-CZ-NH2	7.91	124.25	120.30
1	B	53	LYS	CB-CG-CD	-7.80	91.31	111.60
1	B	341	LYS	CA-CB-CG	7.64	130.22	113.40
1	A	7	PHE	CB-CG-CD1	7.60	126.12	120.80
1	A	286	ASP	CB-CG-OD1	7.57	125.11	118.30
1	B	221	LYS	CB-CG-CD	7.57	131.27	111.60
1	B	297	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	177	LEU	CA-CB-CG	7.46	132.46	115.30
1	B	128	ASN	CB-CA-C	-7.44	95.52	110.40
1	A	482	ARG	CD-NE-CZ	7.40	133.96	123.60
1	B	104	ARG	CD-NE-CZ	7.40	133.96	123.60
1	B	127	MET	C-N-CA	7.37	140.12	121.70
1	A	27	ASP	CB-CG-OD2	7.24	124.81	118.30
1	A	162	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	A	482	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	B	504	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	A	365	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	B	162	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	B	231	GLU	OE1-CD-OE2	-7.10	114.78	123.30
1	B	446	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	B	457	THR	CB-CA-C	-6.93	92.89	111.60
1	A	127	MET	C-N-CA	6.92	138.99	121.70
1	A	244	TYR	CB-CG-CD2	-6.86	116.89	121.00
1	A	104	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	195	MET	CG-SD-CE	-6.67	89.52	100.20
1	B	7	PHE	CB-CG-CD1	6.66	125.47	120.80
1	B	201	GLU	OE1-CD-OE2	6.66	131.29	123.30
1	B	560	LEU	CA-C-O	-6.66	106.12	120.10
1	A	457	THR	CB-CA-C	-6.58	93.85	111.60
1	A	244	TYR	CB-CG-CD1	6.51	124.91	121.00
1	A	526	ARG	NE-CZ-NH2	6.49	123.55	120.30
1	B	552	GLN	CB-CG-CD	6.45	128.36	111.60
1	A	396	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	A	312	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	B	505	THR	CB-CA-C	-6.33	94.50	111.60
1	A	350	ARG	NH1-CZ-NH2	-6.33	112.44	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	B	429	ALA	N-CA-CB	-6.30	101.29	110.10
1	A	494	ASP	CB-CG-OD1	6.18	123.86	118.30
1	B	7	PHE	CB-CG-CD2	-6.13	116.51	120.80
1	B	8	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	A	457	THR	N-CA-CB	6.07	121.83	110.30
1	A	7	PHE	CB-CG-CD2	-6.05	116.57	120.80
1	A	53	LYS	CB-CG-CD	-6.05	95.88	111.60
1	A	552	GLN	CB-CG-CD	6.02	127.25	111.60
1	A	142	VAL	N-CA-CB	-6.00	98.29	111.50
1	B	330	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	B	408	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	B	214	MET	CG-SD-CE	5.90	109.64	100.20
1	A	8	ARG	CA-CB-CG	5.88	126.33	113.40
1	B	286	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	B	177	LEU	CA-CB-CG	5.84	128.74	115.30
1	A	560	LEU	CA-C-O	-5.84	107.83	120.10
1	A	37	VAL	CA-C-O	-5.83	107.85	120.10
1	A	128	ASN	N-CA-CB	-5.83	100.11	110.60
1	B	506	HIS	N-CA-CB	-5.79	100.18	110.60
1	A	505	THR	N-CA-CB	5.79	121.29	110.30
1	B	129	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	B	457	THR	N-CA-CB	5.76	121.25	110.30
1	A	505	THR	CB-CA-C	-5.76	96.05	111.60
1	A	211	ARG	CB-CG-CD	5.74	126.51	111.60
1	B	7	PHE	N-CA-C	5.71	126.41	111.00
1	B	453	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	A	104	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	B	222	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	B	192	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	325	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	B	505	THR	N-CA-CB	5.53	120.80	110.30
1	B	114	ARG	CB-CG-CD	5.46	125.79	111.60
1	B	78	ARG	NE-CZ-NH1	-5.45	117.57	120.30
1	B	493	ASP	CB-CG-OD2	-5.39	113.44	118.30
1	A	48	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	7	PHE	N-CA-C	5.35	125.43	111.00
1	B	142	VAL	N-CA-CB	-5.29	99.86	111.50
1	A	506	HIS	N-CA-CB	-5.27	101.12	110.60
1	B	48	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	170	ASP	CB-CG-OD1	5.23	123.00	118.30
1	A	30	ARG	CB-CG-CD	5.22	125.16	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	LYS	CB-CA-C	-5.20	100.01	110.40
1	B	396	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	A	8	ARG	CB-CG-CD	5.16	125.03	111.60
1	B	264	LYS	CB-CA-C	-5.16	100.07	110.40
1	B	143	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	B	148	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	A	136	GLU	OE1-CD-OE2	-5.11	117.17	123.30
1	B	453	ASP	OD1-CG-OD2	5.11	133.00	123.30
1	A	128	ASN	N-CA-C	5.09	124.75	111.00
1	B	350	ARG	NH1-CZ-NH2	-5.09	113.80	119.40
1	B	128	ASN	N-CA-CB	-5.08	101.45	110.60
1	B	168	VAL	CB-CA-C	-5.08	101.75	111.40
1	B	187	TYR	CA-CB-CG	-5.08	103.75	113.40
1	B	516	THR	CA-CB-CG2	5.06	119.48	112.40
1	B	136	GLU	OE1-CD-OE2	-5.03	117.26	123.30
1	A	325	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	350	ARG	Sidechain
1	B	350	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	4346	0	4288	107	1
1	B	4346	0	4288	107	1
2	A	53	0	31	6	0
2	B	53	0	31	10	0
3	A	11	0	7	2	0
3	B	11	0	8	2	0
4	A	139	0	0	9	0
4	B	117	0	0	3	0
All	All	9076	0	8653	209	1

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 (209) 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)
2:B:600:FAD:H8A	2:B:600:FAD:C5B	1.73	1.17
2:A:600:FAD:H8A	2:A:600:FAD:C5B	1.75	1.15
2:A:600:FAD:C8A	2:A:600:FAD:H51A	1.86	1.04
2:B:600:FAD:H51A	2:B:600:FAD:H8A	1.04	1.03
1:A:349:GLY:H	1:A:352:ASN:HD21	1.09	1.00
2:B:600:FAD:H51A	2:B:600:FAD:C8A	1.90	0.99
2:A:600:FAD:H8A	2:A:600:FAD:H51A	1.00	0.97
1:B:349:GLY:H	1:B:352:ASN:HD21	1.15	0.91
1:B:550:PRO:HB2	1:B:552:GLN:NE2	1.86	0.90
1:A:550:PRO:HB2	1:A:552:GLN:NE2	1.89	0.87
1:A:516:THR:HG21	4:A:2122:HOH:O	1.80	0.79
1:A:149:HIS:HD1	1:A:408:TYR:HH	1.25	0.76
1:B:550:PRO:HB2	1:B:552:GLN:HE22	1.50	0.74
1:A:505:THR:HG21	1:A:513:ILE:HD12	1.68	0.73
1:A:550:PRO:HB2	1:A:552:GLN:HE22	1.53	0.72
1:B:505:THR:HG21	1:B:513:ILE:HD12	1.69	0.71
1:B:102:ILE:HG22	1:B:104:ARG:HG3	1.73	0.71
2:A:600:FAD:C8A	2:A:600:FAD:C5B	2.60	0.70
1:B:552:GLN:NE2	1:B:552:GLN:H	1.90	0.68
1:A:457:THR:HG21	4:A:2082:HOH:O	1.92	0.68
2:B:600:FAD:C8A	2:B:600:FAD:C5B	2.58	0.68
1:A:552:GLN:H	1:A:552:GLN:NE2	1.92	0.67
1:B:521:ASN:O	1:B:522:SER:HB2	1.94	0.67
1:A:79:ASN:ND2	1:A:82:ASP:H	1.91	0.67
1:A:428:ILE:HD11	1:A:503:TYR:HB3	1.75	0.67
2:B:600:FAD:H9	2:B:600:FAD:O2'	1.94	0.67
1:A:443:THR:HG21	1:A:469:VAL:HG21	1.77	0.66
1:A:217:LEU:CD2	1:B:516:THR:HG23	2.26	0.66
1:B:194:TRP:O	1:B:197:HIS:HD2	1.79	0.65
1:A:188:THR:HB	1:A:189:PRO:CD	2.25	0.65
1:A:149:HIS:ND1	1:A:408:TYR:OH	2.17	0.65
1:A:312:ARG:HG2	1:A:457:THR:HG23	1.78	0.64
1:B:79:ASN:ND2	1:B:82:ASP:H	1.95	0.64
1:B:341:LYS:O	1:B:345:GLN:HG3	1.98	0.64
1:B:471:ILE:HG21	1:B:484:VAL:HG13	1.78	0.64
1:B:443:THR:HG21	1:B:469:VAL:HG21	1.81	0.63
1:B:161:ARG:HG3	4:B:2005:HOH:O	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LEU:HD11	1:B:253:LEU:HD21	1.81	0.62
1:A:282:THR:HG22	1:A:352:ASN:ND2	2.15	0.61
1:B:149:HIS:ND1	1:B:408:TYR:OH	2.16	0.61
1:B:149:HIS:CE1	1:B:408:TYR:HE2	2.19	0.61
1:B:310:THR:HG22	1:B:459:THR:HG22	1.82	0.61
1:A:516:THR:HG23	1:B:217:LEU:CD2	2.31	0.61
1:A:531:LEU:HD22	1:B:531:LEU:HD22	1.82	0.61
1:A:189:PRO:HB2	1:A:270:MET:HE3	1.82	0.61
1:B:187:TYR:O	1:B:307:ASN:HB2	2.01	0.60
1:A:167:ASP:OD1	1:A:186:GLY:HA3	2.02	0.59
1:A:478:LEU:H	1:A:478:LEU:HD12	1.67	0.59
1:A:188:THR:CB	1:A:189:PRO:CD	2.81	0.59
1:A:468:ILE:HD11	3:A:601:EUG:H92	1.84	0.59
1:B:188:THR:HB	1:B:189:PRO:CD	2.32	0.59
1:B:357:LEU:HD11	1:B:368:TRP:HB2	1.84	0.59
1:B:478:LEU:H	1:B:478:LEU:HD12	1.67	0.59
1:B:167:ASP:OD1	1:B:186:GLY:HA3	2.03	0.59
1:A:152:HIS:HD2	4:A:2096:HOH:O	1.85	0.58
1:A:149:HIS:CE1	1:A:408:TYR:HE2	2.22	0.58
1:B:516:THR:HG21	4:B:2100:HOH:O	2.02	0.58
1:B:552:GLN:HE21	1:B:552:GLN:H	1.51	0.58
1:B:106:SER:HB2	2:B:600:FAD:HM81	1.86	0.57
1:B:545:LYS:HE2	2:B:600:FAD:O2B	2.04	0.57
1:B:312:ARG:HG2	1:B:457:THR:HG23	1.86	0.57
1:A:332:GLU:HB3	1:A:333:PRO:HD2	1.85	0.57
1:B:149:HIS:HE1	1:B:408:TYR:HE2	1.53	0.57
1:A:57:THR:HG22	1:A:74:ILE:HD11	1.86	0.57
1:A:349:GLY:N	1:A:352:ASN:HD21	1.92	0.57
1:B:188:THR:CB	1:B:189:PRO:CD	2.83	0.57
1:A:552:GLN:HE21	1:A:552:GLN:H	1.50	0.57
1:B:332:GLU:HB3	1:B:333:PRO:HD2	1.87	0.56
1:A:14:PRO:HG3	1:A:558:TRP:CZ2	2.40	0.56
1:A:217:LEU:HD23	1:B:516:THR:HG23	1.86	0.56
1:A:149:HIS:HE1	1:A:408:TYR:HE2	1.53	0.56
1:B:297:ARG:HB3	1:B:298:PRO:CD	2.36	0.56
1:A:102:ILE:HG22	1:A:104:ARG:HG3	1.87	0.55
1:B:189:PRO:HG2	1:B:270:MET:HE1	1.89	0.55
1:A:194:TRP:O	1:A:197:HIS:HD2	1.89	0.55
1:A:102:ILE:HG12	1:A:175:SER:HB2	1.89	0.55
1:B:428:ILE:HD11	1:B:503:TYR:HB3	1.88	0.54
1:B:385:PHE:HB3	1:B:386:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:ILE:HG21	1:A:484:VAL:HG13	1.89	0.54
1:A:505:THR:CG2	1:A:513:ILE:HD12	2.37	0.54
1:A:341:LYS:O	1:A:345:GLN:HG3	2.07	0.54
1:A:513:ILE:O	1:A:516:THR:HB	2.08	0.54
1:B:79:ASN:HD22	1:B:79:ASN:C	2.10	0.54
1:B:505:THR:CG2	1:B:513:ILE:HD12	2.37	0.54
1:A:197:HIS:HE1	1:A:251:ASP:OD2	1.90	0.54
1:A:78:ARG:HB2	1:A:82:ASP:OD2	2.08	0.54
2:B:600:FAD:C9	2:B:600:FAD:O2'	2.56	0.53
1:B:197:HIS:HE1	1:B:251:ASP:OD2	1.91	0.53
4:A:2012:HOH:O	1:B:526:ARG:HB3	2.09	0.53
1:A:385:PHE:HB3	1:A:386:PRO:HD2	1.90	0.53
1:B:357:LEU:CD1	1:B:368:TRP:HB2	2.39	0.53
1:A:7:PHE:HB3	4:A:2002:HOH:O	2.08	0.53
1:A:93:PHE:O	1:A:94:SER:HB2	2.07	0.53
1:A:505:THR:HG23	4:A:2123:HOH:O	2.08	0.52
1:B:79:ASN:HD22	1:B:82:ASP:H	1.57	0.52
1:A:518:ASN:O	1:A:519:TRP:C	2.45	0.52
1:B:513:ILE:O	1:B:516:THR:HB	2.09	0.52
1:B:102:ILE:HG12	1:B:175:SER:HB2	1.90	0.52
1:B:149:HIS:CE1	1:B:408:TYR:CE2	2.97	0.52
1:A:480:GLN:O	1:A:484:VAL:HG23	2.08	0.52
1:A:189:PRO:HG2	1:A:270:MET:HE1	1.91	0.52
1:A:438:MET:HG2	1:A:500:TRP:HH2	1.75	0.52
1:B:106:SER:CB	2:B:600:FAD:HM81	2.39	0.52
1:B:57:THR:HG22	1:B:74:ILE:HD11	1.91	0.51
1:B:417:LEU:HB3	1:B:418:PRO:HD2	1.92	0.51
1:B:14:PRO:HG3	1:B:558:TRP:CZ2	2.46	0.51
1:B:282:THR:HG22	1:B:352:ASN:ND2	2.25	0.51
1:B:468:ILE:HD11	3:B:601:EUG:C9	2.41	0.50
1:A:149:HIS:CE1	1:A:408:TYR:CE2	3.00	0.50
1:A:24:PHE:HD1	1:A:25:ILE:HD12	1.76	0.50
1:A:346:LEU:O	1:A:347:ASN:HB2	2.12	0.50
1:A:521:ASN:O	1:A:522:SER:HB2	2.11	0.49
1:B:516:THR:HG22	1:B:517:TYR:CD1	2.47	0.49
1:B:133:VAL:HG11	1:B:160:LEU:HD13	1.94	0.49
1:B:346:LEU:O	1:B:347:ASN:HB2	2.11	0.49
1:B:480:GLN:O	1:B:484:VAL:HG23	2.12	0.49
2:B:600:FAD:H8A	2:B:600:FAD:H52A	1.83	0.49
1:A:51:TYR:CE1	1:A:104:ARG:HD3	2.48	0.49
1:A:21:PHE:CZ	1:A:25:ILE:HD13	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:VAL:HG11	1:A:160:LEU:HD13	1.95	0.49
1:A:357:LEU:HD11	1:A:368:TRP:HB2	1.94	0.48
1:A:108:TYR:CZ	1:A:504:ARG:HG2	2.48	0.48
1:A:357:LEU:CD1	1:A:368:TRP:HB2	2.44	0.48
1:B:24:PHE:HD1	1:B:25:ILE:HD12	1.78	0.48
1:B:93:PHE:O	1:B:94:SER:HB2	2.14	0.48
1:B:59:ASP:OD2	1:B:62:HIS:HA	2.13	0.48
1:B:518:ASN:O	1:B:519:TRP:C	2.52	0.47
1:A:477:ASP:O	1:A:481:LYS:HG3	2.14	0.47
1:A:63:VAL:HG12	1:A:473:PHE:CZ	2.49	0.47
1:B:297:ARG:HB3	1:B:298:PRO:HD3	1.96	0.47
1:A:387:GLU:HG2	4:A:2091:HOH:O	2.15	0.47
1:A:79:ASN:HD22	1:A:82:ASP:H	1.62	0.47
1:A:79:ASN:HD22	1:A:79:ASN:C	2.18	0.47
1:B:484:VAL:O	1:B:487:LEU:HB3	2.15	0.47
1:A:427:PRO:HA	1:A:502:GLU:HA	1.95	0.47
1:B:438:MET:HG2	1:B:500:TRP:HH2	1.80	0.47
1:A:195:MET:SD	1:B:195:MET:HE1	2.54	0.47
1:A:253:LEU:HD21	1:B:253:LEU:HD11	1.96	0.46
1:A:516:THR:HG23	1:B:217:LEU:HD23	1.97	0.46
1:B:238:ILE:HG22	1:B:238:ILE:O	2.14	0.46
1:B:312:ARG:HD3	1:B:354:TYR:CE1	2.49	0.46
1:A:417:LEU:HB3	1:A:418:PRO:HD2	1.97	0.46
1:B:51:TYR:CE1	1:B:104:ARG:HD3	2.50	0.46
1:B:188:THR:HB	1:B:189:PRO:HD3	1.96	0.46
1:A:519:TRP:CH2	1:B:211:ARG:HD3	2.50	0.46
1:A:253:LEU:CD1	1:B:253:LEU:HD21	2.44	0.46
1:B:468:ILE:HD11	3:B:601:EUG:H93	1.98	0.46
1:A:516:THR:HG22	1:A:517:TYR:CD1	2.50	0.46
1:A:282:THR:HG22	1:A:352:ASN:HD22	1.82	0.45
1:B:131:LEU:HD11	1:B:143:GLU:HG3	1.98	0.45
1:B:24:PHE:CD1	1:B:25:ILE:HD12	2.52	0.45
1:A:244:TYR:OH	1:B:195:MET:HG2	2.16	0.45
1:A:468:ILE:HD11	3:A:601:EUG:C9	2.46	0.45
1:A:56:HIS:HB2	1:A:74:ILE:HD13	1.99	0.45
1:B:21:PHE:CZ	1:B:25:ILE:HD13	2.51	0.45
1:B:31:ILE:HD13	1:B:85:SER:HB3	1.99	0.45
1:A:188:THR:HB	1:A:189:PRO:HD2	1.98	0.45
1:B:78:ARG:HB2	1:B:82:ASP:OD2	2.17	0.45
1:A:24:PHE:CD1	1:A:25:ILE:HD12	2.52	0.45
1:A:361:GLU:HB3	1:A:362:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ALA:HB1	1:B:95:PHE:O	2.18	0.44
1:B:108:TYR:CZ	1:B:504:ARG:HG2	2.52	0.44
1:A:98:TRP:CD2	1:A:113:PRO:HA	2.52	0.44
1:A:275:GLY:HA3	1:A:359:GLY:O	2.17	0.44
1:A:214:MET:SD	1:A:245:GLY:HA2	2.57	0.44
1:A:187:TYR:O	1:A:307:ASN:HB2	2.16	0.44
1:B:114:ARG:NH1	1:B:511:ASP:OD2	2.50	0.44
1:B:112:ALA:O	1:B:507:LEU:HD11	2.17	0.44
1:B:378:ILE:O	1:B:381:VAL:HG12	2.18	0.43
1:A:211:ARG:HG2	1:B:519:TRP:CE3	2.54	0.43
1:A:312:ARG:HD3	1:A:354:TYR:CE1	2.53	0.43
1:A:195:MET:SD	1:B:195:MET:SD	3.17	0.43
1:B:152:HIS:HD2	4:B:2085:HOH:O	2.01	0.43
1:A:195:MET:HG2	1:B:244:TYR:OH	2.19	0.42
1:B:357:LEU:HB3	1:B:364:ARG:HG2	2.01	0.42
1:B:332:GLU:HB3	1:B:333:PRO:CD	2.49	0.42
1:B:98:TRP:CD2	1:B:113:PRO:HA	2.54	0.42
1:A:549:TRP:CH2	1:A:558:TRP:HB3	2.54	0.42
1:A:102:ILE:CG1	1:A:175:SER:HB2	2.48	0.42
1:B:177:LEU:HB2	1:B:265:ILE:HG22	2.01	0.42
1:B:491:LEU:HA	1:B:491:LEU:HD23	1.93	0.42
1:B:385:PHE:HB3	1:B:386:PRO:CD	2.50	0.42
1:B:90:ALA:O	1:B:94:SER:N	2.53	0.42
1:A:387:GLU:HB2	4:A:2091:HOH:O	2.18	0.42
1:B:189:PRO:HB2	1:B:270:MET:HE3	2.02	0.41
1:B:13:PRO:HG3	1:B:95:PHE:CE1	2.55	0.41
1:A:253:LEU:HD21	1:B:253:LEU:CG	2.49	0.41
1:A:28:ILE:O	1:A:32:VAL:HG22	2.20	0.41
1:A:398:ARG:NH1	1:A:410:GLU:OE2	2.50	0.41
1:A:142:VAL:HG22	1:A:146:VAL:HG21	2.02	0.41
1:A:257:SER:HA	4:A:2069:HOH:O	2.20	0.41
1:A:188:THR:HB	1:A:189:PRO:HD3	2.00	0.41
1:A:189:PRO:HG2	1:A:270:MET:CE	2.50	0.41
1:A:195:MET:CE	1:B:195:MET:SD	3.08	0.41
1:A:238:ILE:O	1:A:238:ILE:HG22	2.19	0.41
1:A:310:THR:HG22	1:A:459:THR:HG22	2.03	0.41
1:B:167:ASP:OD1	1:B:193:HIS:NE2	2.54	0.41
1:A:101:SER:O	1:A:124:GLY:HA3	2.20	0.41
1:A:253:LEU:CG	1:B:253:LEU:HD21	2.50	0.41
1:B:95:PHE:CE1	1:B:119:VAL:HG23	2.55	0.41
1:B:361:GLU:N	1:B:362:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:SER:HB2	2:A:600:FAD:HM81	2.03	0.41
1:A:144:PRO:HD3	1:A:263:THR:O	2.21	0.41
2:A:600:FAD:H5'2	2:A:600:FAD:H2'	1.87	0.40
1:B:71:ALA:HB2	1:B:120:VAL:HG23	2.03	0.40
1:B:427:PRO:HA	1:B:502:GLU:HA	2.03	0.40
1:A:425:PHE:CD2	1:A:427:PRO:HD3	2.56	0.40
1:B:51:TYR:CE1	1:B:171:LEU:HD13	2.56	0.40
1:A:417:LEU:O	1:A:418:PRO:C	2.60	0.40

All (1) 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)
1:A:37:VAL:O	1:B:391:GLU:OE2[6_655]	2.01	0.19

## 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	546/560 (98%)	527 (96%)	18 (3%)	1 (0%)	52	69
1	B	546/560 (98%)	524 (96%)	21 (4%)	1 (0%)	52	69
All	All	1092/1120 (98%)	1051 (96%)	39 (4%)	2 (0%)	52	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	418	PRO
1	A	418	PRO

### 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	469/480 (98%)	436 (93%)	33 (7%)	19	29
1	B	469/480 (98%)	433 (92%)	36 (8%)	16	24
All	All	938/960 (98%)	869 (93%)	69 (7%)	17	26

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	8	ARG
1	A	25	ILE
1	A	41	SER
1	A	78	ARG
1	A	79	ASN
1	A	95	PHE
1	A	114	ARG
1	A	128	ASN
1	A	142	VAL
1	A	149	HIS
1	A	177	LEU
1	A	200	MET
1	A	297	ARG
1	A	301	LEU
1	A	314	ILE
1	A	330	ARG
1	A	331	THR
1	A	336	ASP
1	A	344	LYS
1	A	391	GLU
1	A	418	PRO
1	A	432	SER
1	A	448	GLN
1	A	457	THR
1	A	467	HIS
1	A	472	VAL

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Mol	Chain	Res	Type
1	A	478	LEU
1	A	503	TYR
1	A	505	THR
1	A	516	THR
1	A	552	GLN
1	A	554	SER
1	B	7	PHE
1	B	8	ARG
1	B	25	ILE
1	B	41	SER
1	B	78	ARG
1	B	79	ASN
1	B	95	PHE
1	B	114	ARG
1	B	128	ASN
1	B	142	VAL
1	B	149	HIS
1	B	177	LEU
1	B	200	MET
1	B	251	ASP
1	B	297	ARG
1	B	301	LEU
1	B	303	MET
1	B	314	ILE
1	B	329	SER
1	B	330	ARG
1	B	331	THR
1	B	336	ASP
1	B	344	LYS
1	B	412	LYS
1	B	418	PRO
1	B	432	SER
1	B	448	GLN
1	B	457	THR
1	B	467	HIS
1	B	472	VAL
1	B	478	LEU
1	B	503	TYR
1	B	505	THR
1	B	516	THR
1	B	552	GLN
1	B	554	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	128	ASN
1	A	152	HIS
1	A	197	HIS
1	A	240	HIS
1	A	352	ASN
1	A	485	GLN
1	A	520	ASN
1	A	552	GLN
1	B	79	ASN
1	B	128	ASN
1	B	152	HIS
1	B	158	ASN
1	B	197	HIS
1	B	240	HIS
1	B	352	ASN
1	B	520	ASN
1	B	552	GLN
1	B	555	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](#)

4 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	FAD	A	600	-	48,58,58	1.66	7 (14%)	54,89,89	2.45	20 (37%)
3	EUG	A	601	-	11,11,12	0.80	0	14,14,15	2.53	3 (21%)
2	FAD	B	600	-	48,58,58	1.70	8 (16%)	54,89,89	2.22	16 (29%)
3	EUG	B	601	-	11,11,12	0.68	0	14,14,15	2.23	2 (14%)

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	FAD	A	600	-	-	0/30/50/50	0/6/6/6
3	EUG	A	601	-	-	0/4/4/5	0/1/1/1
2	FAD	B	600	-	-	0/30/50/50	0/6/6/6
3	EUG	B	601	-	-	0/4/4/5	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	PA-O2A	-4.82	1.34	1.54
2	A	600	FAD	P-O2P	-4.28	1.36	1.54
2	B	600	FAD	PA-O2A	-4.13	1.37	1.54
2	A	600	FAD	C10-N10	-3.74	1.34	1.39
2	B	600	FAD	C10-N10	-3.43	1.35	1.39
2	B	600	FAD	P-O2P	-3.22	1.41	1.54
2	B	600	FAD	C9A-N10	2.21	1.41	1.38
2	A	600	FAD	C4X-C10	2.49	1.45	1.41
2	A	600	FAD	C4-N3	2.66	1.38	1.33
2	B	600	FAD	C4X-C10	2.81	1.46	1.41
2	B	600	FAD	C4-N3	3.05	1.38	1.33
2	A	600	FAD	O5'-C5'	3.10	1.57	1.44
2	B	600	FAD	O5'-C5'	3.82	1.60	1.44
2	A	600	FAD	O4B-C1B	4.02	1.46	1.41
2	B	600	FAD	O4B-C1B	5.31	1.47	1.41

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	N3A-C2A-N1A	-5.35	124.80	128.89
2	B	600	FAD	C4X-C4-N3	-4.98	116.78	123.59
2	A	600	FAD	C4X-C4-N3	-4.67	117.20	123.59
2	A	600	FAD	C1B-N9A-C4A	-3.94	120.99	126.94
2	B	600	FAD	C1B-N9A-C4A	-3.91	121.04	126.94
2	B	600	FAD	C4B-O4B-C1B	-3.83	105.50	109.72
2	A	600	FAD	C4B-O4B-C1B	-3.69	105.66	109.72
2	B	600	FAD	O5B-PA-O1A	-3.67	95.36	109.62
2	B	600	FAD	C5X-C9A-N10	-3.66	114.84	117.62
2	A	600	FAD	O5B-PA-O1A	-3.22	97.13	109.62
3	A	601	EUG	O3-C3-C2	-3.07	118.96	124.21
2	B	600	FAD	O3P-P-O5'	-2.80	95.51	102.94
2	A	600	FAD	C4-C4X-C10	-2.59	118.29	119.94
2	A	600	FAD	O5'-P-O1P	-2.58	99.59	109.62
2	B	600	FAD	O2'-C2'-C1'	-2.42	103.99	109.94
2	A	600	FAD	O3P-P-O5'	-2.41	96.54	102.94
2	A	600	FAD	C5X-C9A-N10	-2.39	115.80	117.62
2	B	600	FAD	O4B-C4B-C5B	-2.21	101.43	109.32
2	A	600	FAD	O2'-C2'-C1'	-2.10	104.80	109.94
2	B	600	FAD	O5B-C5B-C4B	-2.08	101.46	109.12
2	B	600	FAD	C7-C6-C5X	2.00	124.19	120.92
2	A	600	FAD	C7-C6-C5X	2.06	124.28	120.92
2	A	600	FAD	C4A-C5A-N7A	2.14	111.45	109.48
2	B	600	FAD	O4'-C4'-C3'	2.14	114.40	109.02
2	A	600	FAD	O2A-PA-O1A	2.36	125.31	112.53
2	A	600	FAD	O2P-P-O5'	2.37	120.43	108.46
2	B	600	FAD	C4-C4X-N5	2.54	121.81	118.72
3	B	601	EUG	O3-C3-C4	2.92	118.42	114.57
2	A	600	FAD	C4-C4X-N5	3.07	122.44	118.72
2	A	600	FAD	C2A-N1A-C6A	3.26	124.58	118.77
2	B	600	FAD	C2B-C1B-N9A	3.31	119.35	114.29
2	A	600	FAD	C2B-C1B-N9A	3.68	119.92	114.29
2	B	600	FAD	P-O3P-PA	4.26	144.68	132.73
2	A	600	FAD	P-O3P-PA	4.37	144.99	132.73
3	A	601	EUG	O3-C3-C4	5.69	122.07	114.57
2	B	600	FAD	O3P-PA-O5B	5.70	118.07	102.94
2	B	600	FAD	C4-N3-C2	6.08	120.50	115.25
2	A	600	FAD	O3P-PA-O5B	6.13	119.20	102.94
3	A	601	EUG	C9-O3-C3	6.60	127.56	117.54
2	A	600	FAD	C4-N3-C2	7.29	121.55	115.25
3	B	601	EUG	C9-O3-C3	7.40	128.76	117.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	6	0
3	A	601	EUG	2	0
2	B	600	FAD	10	0
3	B	601	EUG	2	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	550/560 (98%)	-0.37	2 (0%) 93 93	15, 27, 48, 68	15 (2%)
1	B	550/560 (98%)	-0.20	12 (2%) 65 64	15, 27, 48, 68	15 (2%)
All	All	1100/1120 (98%)	-0.28	14 (1%) 79 79	15, 27, 49, 68	30 (2%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	ASN	3.5
1	B	157	ALA	3.4
1	B	49	GLY	3.0
1	B	50	SER	2.9
1	B	51	TYR	2.7
1	B	62	HIS	2.6
1	B	476	LYS	2.5
1	B	52	MET	2.4
1	B	303	MET	2.3
1	A	347	ASN	2.3
1	B	60	PRO	2.3
1	B	159	ASN	2.2
1	B	57	THR	2.0
1	B	331	THR	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
3	EUG	B	601	11/12	0.82	0.19	2.63	25,27,29,30	0
2	FAD	B	600	53/53	0.86	0.19	1.25	32,36,42,43	0
3	EUG	A	601	11/12	0.92	0.21	1.04	25,27,29,29	0
2	FAD	A	600	53/53	0.92	0.17	0.51	32,35,42,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.