



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:29 PM GMT

PDB ID : 1TT0  
Title : Crystal Structure of Pyranose 2-Oxidase  
Authors : Hallberg, B.M.; Leitner, C.; Haltrich, D.; Divne, C.  
Deposited on : 2004-06-21  
Resolution : 1.80 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

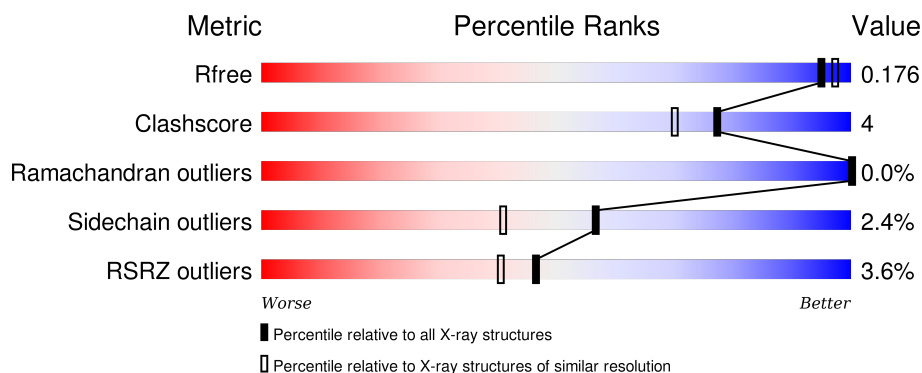
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	623	<div> <div>3%</div> <div>84%</div> <div>9%</div> <div>7%</div> </div>
1	B	623	<div> <div>3%</div> <div>84%</div> <div>8%</div> <div>7%</div> </div>
1	C	623	<div> <div>4%</div> <div>83%</div> <div>9%</div> <div>8%</div> </div>
1	D	623	<div> <div>4%</div> <div>83%</div> <div>9%</div> <div>8%</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	ACT	B	3901	-	-	-	X
2	ACT	C	6901	-	-	-	X
3	FAD	C	6661	-	-	-	X
3	FAD	D	5551	-	-	-	X
4	12P	A	4002	-	-	-	X
4	12P	B	3102	-	-	-	X
4	12P	B	3105	-	-	-	X
4	12P	C	6002	-	-	-	X
4	12P	D	5002	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 21185 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 pyranose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	5	0
			4573	2886	781	881	25			
1	B	577	Total	C	N	O	S	0	4	0
			4566	2882	778	881	25			
1	C	574	Total	C	N	O	S	0	2	0
			4537	2864	778	871	24			
1	D	574	Total	C	N	O	S	0	3	0
			4537	2864	775	874	24			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



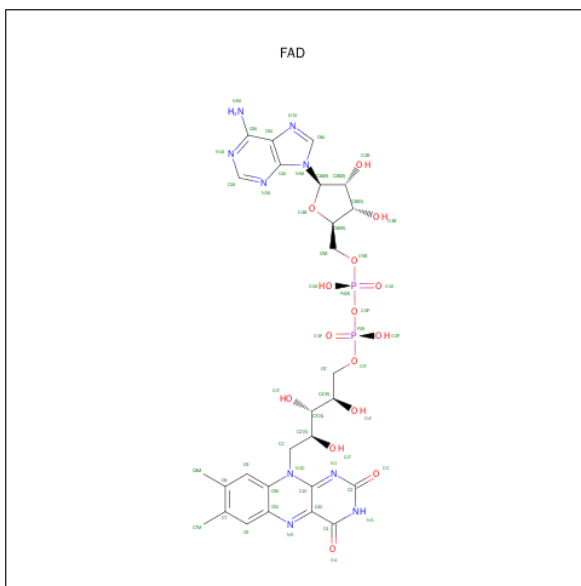
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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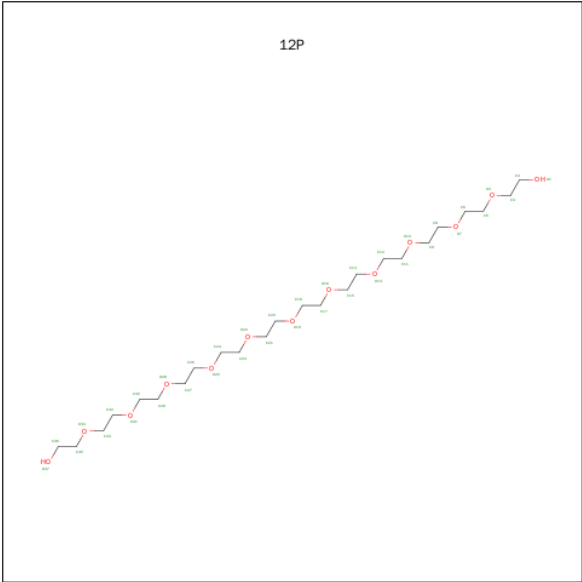
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

- Molecule 4 is DODECAETHYLENE GLYCOL (three-letter code: 12P) (formula:  $C_{24}H_{50}O_{13}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			16	10	6		
4	B	1	Total	C	O	0	0
			12	8	4		
4	B	1	Total	C	O	0	0
			11	7	4		
4	B	1	Total	C	O	0	0
			7	5	2		
4	B	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			12	8	4		
4	A	1	Total	C	O	0	0
			19	12	7		
4	A	1	Total	C	O	0	0
			11	7	4		
4	A	1	Total	C	O	0	0
			9	6	3		
4	A	1	Total	C	O	0	0
			16	10	6		
4	D	1	Total	C	O	0	0
			19	12	7		
4	D	1	Total	C	O	0	0
			11	7	4		
4	D	1	Total	C	O	0	0
			8	5	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			19	13	6		
4	B	1	Total	C	O	0	0
			16	10	6		
4	C	1	Total	C	O	0	0
			13	9	4		
4	C	1	Total	C	O	0	0
			11	7	4		
4	C	1	Total	C	O	0	0
			10	7	3		
4	C	1	Total	C	O	0	0
			14	9	5		

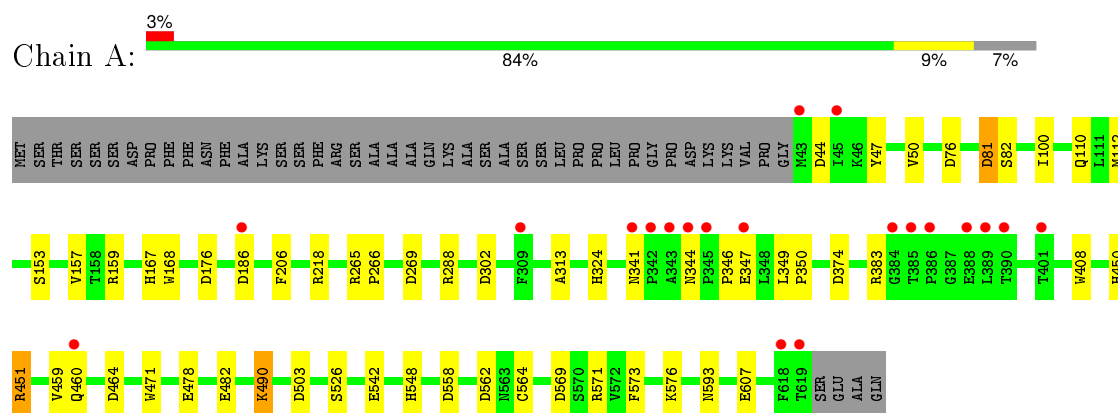
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	674	Total	O	0	0
			674	674		
5	B	671	Total	O	0	0
			671	671		
5	C	543	Total	O	0	1
			544	544		
5	D	607	Total	O	0	0
			607	607		

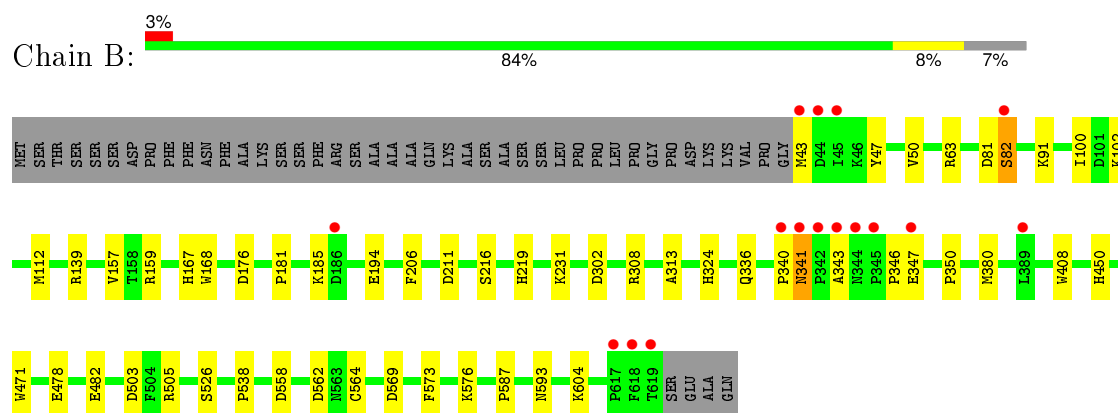
### 3 Residue-property plots

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.

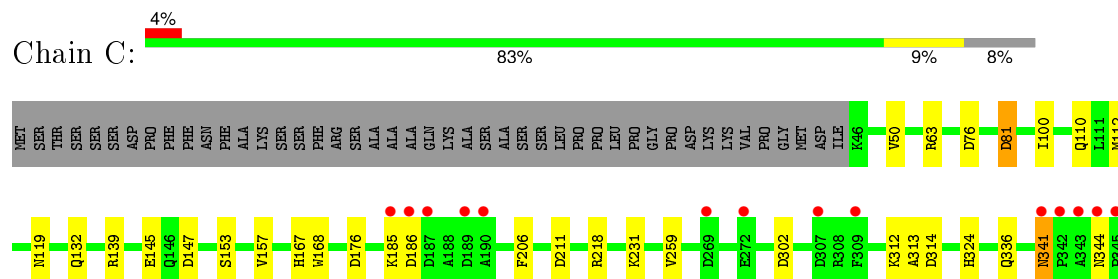
- Molecule 1: pyranose oxidase



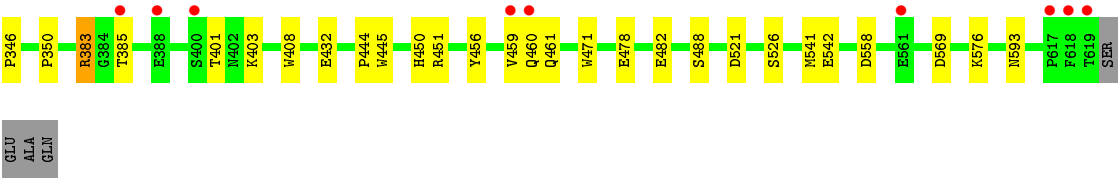
- Molecule 1: pyranose oxidase



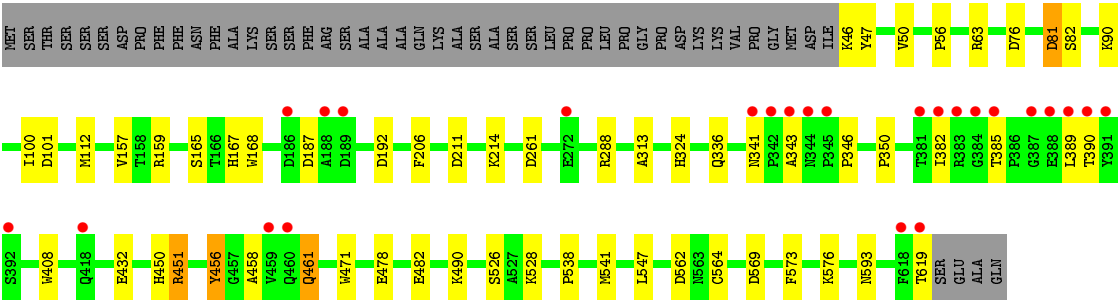
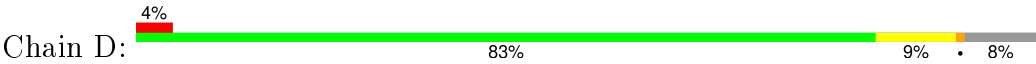
- Molecule 1: pyranose oxidase







● Molecule 1: pyranose oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.92Å 101.69Å 135.63Å 90.00° 90.95° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 38.38 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.6 (30.00-1.80) 92.6 (38.38-1.80)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.134 , 0.171 0.144 , 0.176	Depositor DCC
$R_{free}$ test set	2331 reflections (1.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.1	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 55.3	EDS
Estimated twinning fraction	0.009 for -k,-h,-l 0.007 for k,h,-l 0.017 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 232099 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	21185	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: 12P, FAD, ACT

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	0.92	3/4709 (0.1%)	0.95	19/6402 (0.3%)
1	B	0.94	2/4698 (0.0%)	0.96	18/6388 (0.3%)
1	C	0.86	3/4661 (0.1%)	0.92	15/6338 (0.2%)
1	D	0.91	5/4665 (0.1%)	0.91	13/6344 (0.2%)
All	All	0.91	13/18733 (0.1%)	0.94	65/25472 (0.3%)

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	478	GLU	CD-OE1	8.96	1.35	1.25
1	D	478	GLU	CD-OE1	7.39	1.33	1.25
1	B	482	GLU	CD-OE1	6.98	1.33	1.25
1	D	482	GLU	CD-OE1	6.83	1.33	1.25
1	D	82	SER	CB-OG	6.69	1.50	1.42
1	C	482	GLU	CD-OE1	5.97	1.32	1.25
1	A	482	GLU	CD-OE1	5.93	1.32	1.25
1	C	460	GLN	C-O	5.59	1.33	1.23
1	A	478	GLU	CD-OE1	5.54	1.31	1.25
1	A	383	ARG	CZ-NH1	5.39	1.40	1.33
1	D	63	ARG	CG-CD	-5.37	1.38	1.51
1	C	478	GLU	CD-OE1	5.25	1.31	1.25
1	D	456	TYR	CE1-CZ	5.13	1.45	1.38

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	ASP	CB-CG-OD2	9.90	127.21	118.30
1	C	81	ASP	CB-CG-OD2	9.87	127.18	118.30
1	C	211	ASP	CB-CG-OD1	9.83	127.15	118.30
1	D	81	ASP	CB-CG-OD2	7.83	125.34	118.30
1	C	81	ASP	CB-CG-OD1	-7.73	111.34	118.30
1	B	505	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	81	ASP	CB-CG-OD2	7.56	125.10	118.30
1	A	76	ASP	CB-CG-OD2	7.50	125.05	118.30
1	B	211	ASP	CB-CG-OD1	7.06	124.65	118.30
1	A	558	ASP	CB-CG-OD2	7.01	124.61	118.30
1	C	302	ASP	CB-CG-OD2	6.96	124.56	118.30
1	A	383	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	B	81	ASP	CB-CG-OD1	-6.80	112.17	118.30
1	C	76	ASP	CB-CG-OD2	6.79	124.41	118.30
1	A	383	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	C	186	ASP	CB-CG-OD2	6.49	124.14	118.30
1	C	383	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	A	159	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	269	ASP	CB-CG-OD2	6.30	123.97	118.30
1	D	159	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	A	288	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	569	ASP	CB-CG-OD2	6.17	123.86	118.30
1	B	102	LYS	CD-CE-NZ	-6.16	97.54	111.70
1	D	187	ASP	CB-CG-OD2	6.09	123.78	118.30
1	D	211	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	302	ASP	CB-CG-OD2	5.98	123.69	118.30
1	B	569	ASP	CB-CG-OD2	5.94	123.64	118.30
1	C	176	ASP	CB-CG-OD2	5.93	123.64	118.30
1	D	569	ASP	CB-CG-OD2	5.89	123.60	118.30
1	D	76	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	562	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	503	ASP	CB-CG-OD2	5.78	123.50	118.30
1	C	521	ASP	CB-CG-OD2	5.77	123.49	118.30
1	B	380	MET	CG-SD-CE	-5.77	90.97	100.20
1	B	558	ASP	CB-CG-OD2	5.75	123.47	118.30
1	B	505	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	D	288	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	44	ASP	CB-CG-OD2	5.64	123.37	118.30
1	D	562	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	451[A]	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	451[B]	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	D	101	ASP	CB-CG-OD2	5.54	123.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	D	159	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	349	LEU	CB-CG-CD2	5.47	120.30	111.00
1	A	176	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	562	ASP	CB-CG-OD2	5.42	123.17	118.30
1	B	159	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	503	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	139	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	302	ASP	CB-CG-OD1	5.33	123.09	118.30
1	C	569	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	63	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	C	558	ASP	CB-CG-OD2	5.25	123.02	118.30
1	D	192	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	261	ASP	CB-CG-OD1	5.19	122.97	118.30
1	D	451	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	C	460	GLN	CA-C-N	-5.14	105.90	117.20
1	C	139	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	314	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	147	ASP	CB-CG-OD1	5.06	122.85	118.30
1	A	464	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	63	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	186	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	176	ASP	CB-CG-OD2	5.03	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	460	GLN	Peptide

## 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	4573	0	4411	27	0
1	B	4566	0	4402	25	0
1	C	4537	0	4382	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4537	0	4376	40	0
2	A	4	0	3	1	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
3	A	53	0	29	4	0
3	B	53	0	31	7	0
3	C	53	0	29	0	0
3	D	53	0	30	11	0
4	A	67	0	82	12	0
4	B	72	0	84	10	0
4	C	48	0	52	11	0
4	D	61	0	72	14	0
5	A	674	0	0	8	1
5	B	671	0	0	11	1
5	C	544	0	0	5	0
5	D	607	0	0	6	0
All	All	21185	0	17992	137	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 4.

All (137) 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:A:167:HIS:NE2	3:A:3331:FAD:C8M	1.70	1.55
1:B:167:HIS:HE2	3:B:4441:FAD:C8M	0.89	1.52
1:D:167:HIS:HE2	3:D:5551:FAD:C8M	0.89	1.51
1:D:167:HIS:NE2	3:D:5551:FAD:HM82	0.89	1.21
1:B:167:HIS:CD2	3:B:4441:FAD:HM82	1.80	1.17
1:B:167:HIS:NE2	3:B:4441:FAD:HM82	0.84	1.15
1:D:167:HIS:CD2	3:D:5551:FAD:HM82	1.92	1.05
1:C:576:LYS:NZ	4:C:6002:12P:C17	2.23	1.01
1:B:167:HIS:HE2	3:B:4441:FAD:HM81	1.27	1.00
1:A:576:LYS:NZ	4:A:4002:12P:H21	1.79	0.98
1:B:167:HIS:CE1	3:B:4441:FAD:HM82	2.02	0.94
1:D:167:HIS:CE1	3:D:5551:FAD:HM82	2.02	0.92
1:A:110:GLN:HE21	1:A:167:HIS:HD1	1.16	0.89
1:D:576:LYS:NZ	4:D:5002:12P:H171	1.88	0.88
1:D:167:HIS:HE2	3:D:5551:FAD:HM81	1.33	0.88
1:C:576:LYS:HE2	4:C:6002:12P:O13	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:LYS:HZ3	4:A:4002:12P:H21	1.36	0.86
1:C:576:LYS:CE	4:C:6002:12P:C17	2.53	0.86
1:C:401:THR:HG23	5:C:7169:HOH:O	1.78	0.83
1:C:110:GLN:HE21	1:C:167:HIS:HD1	1.26	0.82
1:C:576:LYS:HE3	4:C:6002:12P:C17	2.08	0.82
1:D:576:LYS:HZ3	4:D:5002:12P:H171	1.46	0.80
1:B:167:HIS:NE2	3:B:4441:FAD:C8M	1.73	0.79
1:A:167:HIS:NE2	3:A:3331:FAD:HM81	1.95	0.79
1:A:167:HIS:CD2	3:A:3331:FAD:C8M	2.66	0.79
4:A:4002:12P:H112	5:A:5184:HOH:O	1.90	0.72
1:C:576:LYS:HZ2	4:C:6002:12P:C17	2.02	0.71
1:C:576:LYS:HZ1	4:C:6002:12P:C17	2.02	0.71
1:D:576:LYS:HE2	4:D:5002:12P:H152	1.74	0.70
1:D:461:GLN:OE1	5:D:6473:HOH:O	2.08	0.70
1:B:82:SER:O	5:B:6642:HOH:O	2.11	0.68
1:A:576:LYS:HZ2	4:A:4002:12P:H21	1.58	0.68
1:D:167:HIS:NE2	3:D:5551:FAD:C8M	1.75	0.66
1:A:374:ASP:OD1	5:A:5575:HOH:O	2.13	0.66
4:B:3101:12P:H22	5:B:6496:HOH:O	1.94	0.66
4:B:3105:12P:H241	5:B:6443:HOH:O	1.95	0.66
4:B:6001:12P:O4	5:B:6442:HOH:O	2.14	0.65
4:B:3103:12P:H91	5:B:6634:HOH:O	1.95	0.65
1:C:231:LYS:NZ	5:C:7258:HOH:O	2.31	0.64
1:C:451[B]:ARG:NH2	1:C:459:VAL:HG21	2.14	0.63
1:D:528:LYS:NZ	5:D:6425:HOH:O	2.01	0.63
1:B:308:ARG:NE	5:B:6508:HOH:O	2.23	0.62
1:A:571:ARG:NH1	4:A:4002:12P:H52	2.15	0.61
1:D:167:HIS:HE2	3:D:5551:FAD:C8	1.96	0.61
1:D:490:LYS:HD3	5:D:6265:HOH:O	2.01	0.60
1:D:458:ALA:O	4:D:5003:12P:O4	2.22	0.58
1:C:157:VAL:HG21	1:C:324:HIS:HE1	1.69	0.58
1:D:336:GLN:HE22	1:D:341:ASN:H	1.51	0.58
1:D:576:LYS:CD	4:D:5002:12P:H22	2.33	0.57
1:A:167:HIS:CE1	3:A:3331:FAD:C8M	2.76	0.57
1:D:167:HIS:NE2	3:D:5551:FAD:HM81	2.04	0.57
1:D:576:LYS:HD3	4:D:5002:12P:H52	1.87	0.57
1:D:167:HIS:CE1	3:D:5551:FAD:C8M	2.74	0.56
1:D:50:VAL:HG13	1:D:313:ALA:HB2	1.86	0.56
1:A:576:LYS:HZ2	4:A:4002:12P:C2	2.18	0.56
1:B:167:HIS:CE1	3:B:4441:FAD:C8M	2.75	0.55
1:D:167:HIS:NE2	3:D:5551:FAD:C8	2.64	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:VAL:HG21	1:A:324:HIS:HE1	1.71	0.55
1:B:50:VAL:HG13	1:B:313:ALA:HB2	1.88	0.55
1:D:81:ASP:OD2	1:D:90:LYS:NZ	2.37	0.54
1:C:576:LYS:HG2	4:C:6002:12P:H82	1.90	0.54
4:A:5001:12P:H31	4:A:5001:12P:O7	2.06	0.54
1:C:461:GLN:HG3	5:C:6945:HOH:O	2.09	0.53
4:A:4002:12P:O19	4:A:4002:12P:H81	2.09	0.53
4:A:4003:12P:C14	5:A:5626:HOH:O	2.56	0.53
1:B:91:LYS:HD2	1:B:100:ILE:HD11	1.91	0.52
4:B:3101:12P:O4	5:B:6496:HOH:O	2.19	0.52
1:D:456:TYR:HB2	4:D:5003:12P:H122	1.91	0.52
4:B:3103:12P:C5	5:B:6634:HOH:O	2.58	0.52
1:C:50:VAL:HG13	1:C:313:ALA:HB2	1.91	0.52
4:B:3103:12P:H52	5:B:6634:HOH:O	2.09	0.51
4:D:5003:12P:H91	5:D:6448:HOH:O	2.09	0.51
1:B:336:GLN:HE21	1:B:340:PRO:HA	1.75	0.51
1:A:218:ARG:HD2	5:A:5028:HOH:O	2.11	0.51
1:D:346:PRO:HG2	1:D:350:PRO:HA	1.93	0.51
4:A:4002:12P:C12	5:A:5602:HOH:O	2.57	0.51
1:C:132:GLN:HG2	5:C:7097:HOH:O	2.10	0.51
1:B:194[A]:GLU:OE2	1:B:604:LYS:NZ	2.31	0.50
1:C:119:ASN:ND2	1:D:461:GLN:HB3	2.27	0.50
1:B:346:PRO:HG2	1:B:350:PRO:HA	1.92	0.50
1:C:346:PRO:HG2	1:C:350:PRO:HA	1.94	0.50
1:A:81:ASP:C	1:A:81:ASP:OD1	2.49	0.49
1:A:576:LYS:NZ	4:A:4002:12P:C2	2.63	0.49
1:D:382:ILE:HD13	5:D:6327:HOH:O	2.13	0.48
1:C:336:GLN:HE22	1:C:341:ASN:H	1.60	0.48
1:D:541:MET:CE	4:D:5003:12P:H111	2.43	0.48
1:D:157:VAL:HG21	1:D:324:HIS:HE1	1.78	0.48
1:C:81:ASP:C	1:C:81:ASP:OD1	2.46	0.48
1:C:576:LYS:HG2	4:C:6002:12P:C8	2.44	0.48
1:B:181:PRO:HG3	1:B:587:PRO:HD2	1.96	0.47
4:D:5003:12P:C9	5:D:6448:HOH:O	2.62	0.47
1:A:346:PRO:HG2	1:A:350:PRO:HA	1.96	0.47
1:A:50:VAL:HG13	1:A:313:ALA:HB2	1.97	0.47
1:D:564:CYS:HG	1:D:573:PHE:HE2	1.61	0.46
1:D:576:LYS:HD3	4:D:5002:12P:H22	1.98	0.46
1:D:432[A]:GLU:HB3	1:D:451:ARG:HB2	1.97	0.45
1:B:47:TYR:O	1:B:313:ALA:HA	2.16	0.45
1:B:336:GLN:NE2	1:B:340:PRO:HA	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:VAL:HG21	1:B:324:HIS:HE1	1.83	0.44
4:C:6004:12P:H142	4:C:6004:12P:H112	1.55	0.44
1:B:576:LYS:HG2	4:B:3102:12P:H82	1.99	0.44
1:A:548:HIS:NE2	2:A:4901:ACT:O	2.51	0.44
1:A:564:CYS:HG	1:A:573:PHE:HE2	1.66	0.43
1:D:56:PRO:HD3	1:D:165:SER:HB3	2.01	0.43
1:A:153:SER:OG	1:A:542:GLU:HG3	2.17	0.43
1:D:576:LYS:CE	4:D:5002:12P:H171	2.48	0.43
1:A:47:TYR:O	1:A:313:ALA:HA	2.18	0.43
1:B:471:TRP:CH2	1:B:526:SER:HA	2.53	0.43
1:A:607:GLU:HG3	5:A:5493:HOH:O	2.19	0.43
1:A:451[A]:ARG:NH2	1:A:459:VAL:HG21	2.34	0.43
1:C:153:SER:OG	1:C:542:GLU:HG3	2.20	0.42
1:B:341:ASN:HD21	1:B:343:ALA:HB3	1.83	0.42
1:C:456:TYR:HB2	4:C:6003:12P:H122	2.01	0.42
1:D:471:TRP:CH2	1:D:526:SER:HA	2.54	0.42
1:A:265:ARG:HA	1:A:266:PRO:C	2.40	0.42
1:D:576:LYS:HZ1	4:D:5002:12P:H171	1.80	0.42
1:B:538:PRO:HG2	1:D:538:PRO:HG2	2.01	0.42
4:B:3105:12P:C24	5:B:6443:HOH:O	2.61	0.42
4:B:3102:12P:H122	5:B:6671:HOH:O	2.19	0.42
1:D:576:LYS:HE2	4:D:5002:12P:C15	2.48	0.41
1:B:564:CYS:HG	1:B:573:PHE:HE2	1.68	0.41
1:B:216:SER:HB3	1:B:219:HIS:HB3	2.02	0.41
1:C:444:PRO:HD2	1:C:445:TRP:CZ3	2.55	0.41
1:D:47:TYR:O	1:D:313:ALA:HA	2.20	0.41
1:D:547:LEU:CD1	3:D:5551:FAD:HM83	2.51	0.41
1:C:432[A]:GLU:HB3	1:C:451[A]:ARG:HB2	2.03	0.41
1:D:341:ASN:HD21	1:D:343:ALA:HB3	1.86	0.41
1:C:63:ARG:HD2	1:C:259:VAL:O	2.21	0.41
1:A:471:TRP:CH2	1:A:526:SER:HA	2.55	0.41
1:C:541:MET:HE1	4:C:6003:12P:H122	2.03	0.40
1:C:145:GLU:HG3	1:C:488:SER:HB2	2.04	0.40
1:C:218:ARG:HD2	5:C:6962:HOH:O	2.20	0.40
4:A:4003:12P:H91	4:A:4003:12P:H121	1.86	0.40
1:C:471:TRP:CH2	1:C:526:SER:HA	2.56	0.40
1:B:347:GLU:CD	1:B:347:GLU:H	2.25	0.40
1:A:82:SER:HB2	5:A:5139:HOH:O	2.21	0.40
1:A:490:LYS:NZ	5:A:5615:HOH:O	2.22	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)
5:A:5652:HOH:O	5:B:6648:HOH:O[2_557]	2.03	0.17

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	580/623 (93%)	565 (97%)	15 (3%)	0	100	100
1	B	579/623 (93%)	566 (98%)	12 (2%)	1 (0%)	52	35
1	C	574/623 (92%)	559 (97%)	15 (3%)	0	100	100
1	D	575/623 (92%)	559 (97%)	16 (3%)	0	100	100
All	All	2308/2492 (93%)	2249 (97%)	58 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	82	SER

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	510/542 (94%)	499 (98%)	11 (2%)	60	45
1	B	509/542 (94%)	499 (98%)	10 (2%)	63	49
1	C	504/542 (93%)	490 (97%)	14 (3%)	51	35
1	D	505/542 (93%)	491 (97%)	14 (3%)	51	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2028/2168 (94%)	1979 (98%)	49 (2%)	57 41

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ILE
1	A	112	MET
1	A	168	TRP
1	A	206	PHE
1	A	341	ASN
1	A	344	ASN
1	A	347	GLU
1	A	408	TRP
1	A	450	HIS
1	A	490	LYS
1	A	593	ASN
1	B	43	MET
1	B	112	MET
1	B	168	TRP
1	B	185	LYS
1	B	206	PHE
1	B	231	LYS
1	B	341	ASN
1	B	408	TRP
1	B	450	HIS
1	B	593	ASN
1	C	100	ILE
1	C	112	MET
1	C	168	TRP
1	C	185	LYS
1	C	206	PHE
1	C	312	LYS
1	C	341	ASN
1	C	344	ASN
1	C	383	ARG
1	C	385	THR
1	C	403	LYS
1	C	408	TRP
1	C	450	HIS
1	C	593	ASN
1	D	46	LYS
1	D	100	ILE

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Mol	Chain	Res	Type
1	D	112	MET
1	D	168	TRP
1	D	206	PHE
1	D	214	LYS
1	D	385	THR
1	D	389	LEU
1	D	390	THR
1	D	408	TRP
1	D	450	HIS
1	D	461	GLN
1	D	593	ASN
1	D	619	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	GLN
1	A	341	ASN
1	A	460	GLN
1	B	132	GLN
1	B	263	GLN
1	B	336	GLN
1	B	341	ASN
1	B	461	GLN
1	C	336	GLN
1	C	341	ASN
1	C	460	GLN
1	D	336	GLN
1	D	341	ASN
1	D	460	GLN
1	D	461	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

28 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$
3	FAD	A	3331	-	48,58,58	1.28	7 (14%)	54,89,89	3.27	15 (27%)
4	12P	A	4001	-	11,11,36	0.48	0	10,10,35	0.42	0
4	12P	A	4002	-	18,18,36	0.51	0	17,17,35	0.33	0
4	12P	A	4003	-	10,10,36	0.52	0	9,9,35	0.21	0
4	12P	A	4004	-	8,8,36	0.52	0	7,7,35	0.20	0
2	ACT	A	4901	-	1,3,3	0.24	0	0,3,3	0.00	-
4	12P	A	5001	-	15,15,36	0.58	0	14,14,35	0.52	0
4	12P	B	3101	-	15,15,36	0.45	0	14,14,35	0.50	0
4	12P	B	3102	-	11,11,36	0.54	0	10,10,35	0.15	0
4	12P	B	3103	-	10,10,36	0.64	0	9,9,35	0.20	0
4	12P	B	3104	-	6,6,36	0.63	0	5,5,35	0.14	0
4	12P	B	3105	-	9,9,36	0.39	0	8,8,35	0.33	0
2	ACT	B	3901	-	1,3,3	0.27	0	0,3,3	0.00	-
3	FAD	B	4441	-	48,58,58	1.34	5 (10%)	54,89,89	3.37	17 (31%)
4	12P	B	6001	-	15,15,36	0.50	0	14,14,35	0.47	0
4	12P	C	6002	-	12,12,36	0.59	0	11,11,35	0.18	0
4	12P	C	6003	-	10,10,36	0.45	0	9,9,35	0.25	0
4	12P	C	6004	-	9,9,36	0.62	0	8,8,35	0.24	0
4	12P	C	6005	-	13,13,36	0.53	0	12,12,35	0.33	0
3	FAD	C	6661	-	48,58,58	1.09	3 (6%)	54,89,89	3.67	19 (35%)
2	ACT	C	6901	-	1,3,3	0.27	0	0,3,3	0.00	-
4	12P	D	4101	-	3,3,36	0.67	0	2,2,35	0.05	0
4	12P	D	5002	-	18,18,36	0.59	0	17,17,35	0.35	0
4	12P	D	5003	-	10,10,36	0.68	0	9,9,35	0.26	0
4	12P	D	5004	-	7,7,36	0.52	0	6,6,35	0.21	0
4	12P	D	5005	-	18,18,36	0.54	0	17,17,35	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	FAD	D	5551	-	48,58,58	1.22	6 (12%)	54,89,89	3.20	14 (25%)
2	ACT	D	5901	-	1,3,3	1.03	0	0,3,3	0.00	-

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
3	FAD	A	3331	-	-	0/30/50/50	0/6/6/6
4	12P	A	4001	-	-	0/9/9/34	0/0/0/0
4	12P	A	4002	-	-	0/16/16/34	0/0/0/0
4	12P	A	4003	-	-	0/8/8/34	0/0/0/0
4	12P	A	4004	-	-	0/6/6/34	0/0/0/0
2	ACT	A	4901	-	-	0/0/0/0	0/0/0/0
4	12P	A	5001	-	-	0/13/13/34	0/0/0/0
4	12P	B	3101	-	-	0/13/13/34	0/0/0/0
4	12P	B	3102	-	-	0/9/9/34	0/0/0/0
4	12P	B	3103	-	-	0/8/8/34	0/0/0/0
4	12P	B	3104	-	-	0/4/4/34	0/0/0/0
4	12P	B	3105	-	-	0/7/7/34	0/0/0/0
2	ACT	B	3901	-	-	0/0/0/0	0/0/0/0
3	FAD	B	4441	-	-	0/30/50/50	0/6/6/6
4	12P	B	6001	-	-	0/13/13/34	0/0/0/0
4	12P	C	6002	-	-	0/10/10/34	0/0/0/0
4	12P	C	6003	-	-	0/8/8/34	0/0/0/0
4	12P	C	6004	-	-	0/7/7/34	0/0/0/0
4	12P	C	6005	-	-	0/11/11/34	0/0/0/0
3	FAD	C	6661	-	-	0/30/50/50	0/6/6/6
2	ACT	C	6901	-	-	0/0/0/0	0/0/0/0
4	12P	D	4101	-	-	0/1/1/34	0/0/0/0
4	12P	D	5002	-	-	0/16/16/34	0/0/0/0
4	12P	D	5003	-	-	0/8/8/34	0/0/0/0
4	12P	D	5004	-	-	0/5/5/34	0/0/0/0
4	12P	D	5005	-	-	0/16/16/34	0/0/0/0
3	FAD	D	5551	-	-	0/30/50/50	0/6/6/6
2	ACT	D	5901	-	-	0/0/0/0	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3331	FAD	C2B-C3B	-2.81	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5551	FAD	O4B-C4B	-2.77	1.38	1.45
3	A	3331	FAD	O3B-C3B	-2.37	1.37	1.43
3	D	5551	FAD	O3B-C3B	-2.27	1.37	1.43
3	A	3331	FAD	O4B-C4B	-2.18	1.40	1.45
3	B	4441	FAD	O4B-C4B	-2.13	1.40	1.45
3	C	6661	FAD	C2B-C3B	-2.00	1.47	1.53
3	B	4441	FAD	C4-N3	2.12	1.37	1.33
3	D	5551	FAD	C4-N3	2.17	1.37	1.33
3	A	3331	FAD	C4X-N5	2.21	1.36	1.33
3	C	6661	FAD	C2A-N1A	2.23	1.38	1.33
3	A	3331	FAD	C1'-N10	2.25	1.50	1.48
3	A	3331	FAD	C2A-N3A	2.36	1.36	1.32
3	D	5551	FAD	C5X-N5	2.47	1.39	1.35
3	B	4441	FAD	C5'-C4'	2.47	1.55	1.51
3	D	5551	FAD	C4X-N5	2.60	1.37	1.33
3	B	4441	FAD	O4B-C1B	2.87	1.44	1.41
3	C	6661	FAD	C4-C4X	2.93	1.47	1.41
3	D	5551	FAD	C4-C4X	3.01	1.47	1.41
3	A	3331	FAD	C4-C4X	3.12	1.47	1.41
3	B	4441	FAD	C4-C4X	3.78	1.48	1.41

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5551	FAD	N3A-C2A-N1A	-14.91	117.47	128.89
3	B	4441	FAD	N3A-C2A-N1A	-14.56	117.75	128.89
3	C	6661	FAD	N3A-C2A-N1A	-14.12	118.08	128.89
3	A	3331	FAD	N3A-C2A-N1A	-13.65	118.45	128.89
3	C	6661	FAD	C4-C4X-C10	-7.84	114.92	119.94
3	B	4441	FAD	C4-C4X-C10	-6.47	115.80	119.94
3	C	6661	FAD	C4X-C4-N3	-6.40	114.83	123.59
3	A	3331	FAD	C4-C4X-C10	-5.95	116.14	119.94
3	B	4441	FAD	C4X-C4-N3	-5.45	116.14	123.59
3	A	3331	FAD	C4X-C4-N3	-5.34	116.28	123.59
3	D	5551	FAD	C4X-C4-N3	-5.17	116.52	123.59
3	D	5551	FAD	C4X-C10-N10	-4.32	117.97	120.52
3	B	4441	FAD	C4B-O4B-C1B	-4.18	105.13	109.72
3	D	5551	FAD	C4-C4X-C10	-4.05	117.35	119.94
3	C	6661	FAD	C4B-O4B-C1B	-3.88	105.46	109.72
3	C	6661	FAD	C4X-C10-N10	-3.36	118.54	120.52
3	B	4441	FAD	C4A-C5A-N7A	-2.84	106.86	109.48
3	A	3331	FAD	C4B-O4B-C1B	-2.73	106.72	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5551	FAD	C9A-C5X-N5	-2.43	118.76	122.36
3	C	6661	FAD	O3'-C3'-C4'	-2.37	102.79	108.75
3	B	4441	FAD	C6-C7-C8	-2.23	115.78	120.04
3	D	5551	FAD	C5B-C4B-C3B	2.02	123.23	115.21
3	A	3331	FAD	C4X-N5-C5X	2.04	119.11	116.76
3	B	4441	FAD	C5B-C4B-C3B	2.09	123.50	115.21
3	A	3331	FAD	C5B-C4B-C3B	2.09	123.51	115.21
3	C	6661	FAD	O2'-C2'-C1'	2.10	115.11	109.94
3	B	4441	FAD	O4B-C1B-N9A	2.22	112.74	108.10
3	B	4441	FAD	O2B-C2B-C3B	2.22	119.06	111.83
3	A	3331	FAD	O2B-C2B-C3B	2.23	119.07	111.83
3	C	6661	FAD	O2'-C2'-C3'	2.25	114.67	109.02
3	B	4441	FAD	C5X-C9A-N10	2.26	119.34	117.62
3	D	5551	FAD	O4B-C4B-C3B	2.31	109.80	105.15
3	C	6661	FAD	C4X-N5-C5X	2.31	119.42	116.76
3	A	3331	FAD	O4B-C1B-N9A	2.32	112.96	108.10
3	A	3331	FAD	C4-C4X-N5	2.36	121.58	118.72
3	C	6661	FAD	O2A-PA-O3P	2.40	116.00	105.09
3	D	5551	FAD	O4B-C1B-N9A	2.42	113.16	108.10
3	B	4441	FAD	C2A-N1A-C6A	2.49	123.22	118.77
3	D	5551	FAD	O2B-C2B-C3B	2.53	120.04	111.83
3	B	4441	FAD	C4X-N5-C5X	2.57	119.72	116.76
3	A	3331	FAD	O4B-C4B-C3B	2.79	110.77	105.15
3	B	4441	FAD	O4B-C4B-C3B	2.90	110.99	105.15
3	C	6661	FAD	O2B-C2B-C3B	2.90	121.26	111.83
3	C	6661	FAD	O4B-C4B-C5B	2.95	119.88	109.32
3	C	6661	FAD	C2A-N1A-C6A	3.18	124.44	118.77
3	B	4441	FAD	C4-C4X-N5	3.19	122.60	118.72
3	C	6661	FAD	O3B-C3B-C4B	3.35	121.10	111.05
3	C	6661	FAD	O4B-C4B-C3B	3.43	112.06	105.15
3	A	3331	FAD	C2A-N1A-C6A	3.49	125.00	118.77
3	C	6661	FAD	O4B-C1B-N9A	3.55	115.53	108.10
3	A	3331	FAD	O3B-C3B-C4B	3.80	122.46	111.05
3	D	5551	FAD	O3B-C3B-C4B	3.84	122.56	111.05
3	D	5551	FAD	C1'-N10-C9A	3.87	123.20	118.86
3	B	4441	FAD	C1'-N10-C9A	3.90	123.24	118.86
3	C	6661	FAD	C1'-N10-C9A	4.27	123.66	118.86
3	D	5551	FAD	C2A-N1A-C6A	4.34	126.52	118.77
3	B	4441	FAD	C2B-C1B-N9A	5.29	122.38	114.29
3	A	3331	FAD	C1'-N10-C9A	5.63	125.19	118.86
3	C	6661	FAD	C2B-C1B-N9A	5.96	123.40	114.29
3	A	3331	FAD	C2B-C1B-N9A	7.06	125.08	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5551	FAD	C2B-C1B-N9A	7.66	126.00	114.29
3	D	5551	FAD	C4-N3-C2	9.53	123.49	115.25
3	A	3331	FAD	C4-N3-C2	11.72	125.38	115.25
3	B	4441	FAD	C4-N3-C2	12.94	126.43	115.25
3	C	6661	FAD	C4-N3-C2	14.96	128.18	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 70 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3331	FAD	4	0
4	A	4002	12P	9	0
4	A	4003	12P	2	0
2	A	4901	ACT	1	0
4	A	5001	12P	1	0
4	B	3101	12P	2	0
4	B	3102	12P	2	0
4	B	3103	12P	3	0
4	B	3105	12P	2	0
3	B	4441	FAD	7	0
4	B	6001	12P	1	0
4	C	6002	12P	8	0
4	C	6003	12P	2	0
4	C	6004	12P	1	0
4	D	5002	12P	9	0
4	D	5003	12P	5	0
3	D	5551	FAD	11	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	577/623 (92%)	-0.16	20 (3%) 48 42	5, 10, 24, 52	0
1	B	577/623 (92%)	-0.21	16 (2%) 56 51	5, 9, 23, 57	0
1	C	574/623 (92%)	-0.03	23 (4%) 42 36	8, 14, 28, 57	0
1	D	574/623 (92%)	-0.07	25 (4%) 38 32	6, 11, 26, 51	0
All	All	2302/2492 (92%)	-0.12	84 (3%) 46 40	5, 11, 25, 57	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	343	ALA	11.2
1	D	343	ALA	9.6
1	A	619	THR	9.5
1	C	343	ALA	8.3
1	C	619	THR	7.0
1	D	389	LEU	6.8
1	B	619	THR	6.6
1	B	344	ASN	6.4
1	D	390	THR	6.4
1	B	342	PRO	6.0
1	A	344	ASN	6.0
1	A	345	PRO	6.0
1	A	343	ALA	5.9
1	A	385	THR	5.7
1	C	345	PRO	5.7
1	D	388	GLU	5.6
1	B	345	PRO	5.6
1	D	342	PRO	5.6
1	C	344	ASN	5.5
1	B	44	ASP	5.4
1	D	618	PHE	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	618	PHE	5.2
1	D	345	PRO	4.9
1	D	186	ASP	4.8
1	D	385	THR	4.8
1	D	344	ASN	4.7
1	A	384	GLY	4.5
1	D	383	ARG	4.3
1	A	342	PRO	4.2
1	D	619	THR	4.2
1	B	341	ASN	4.1
1	C	342	PRO	4.0
1	B	43	MET	4.0
1	A	388	GLU	3.9
1	D	341	ASN	3.9
1	C	385	THR	3.9
1	D	384	GLY	3.8
1	D	382	ILE	3.8
1	D	460	GLN	3.5
1	C	400	SER	3.4
1	B	347	GLU	3.3
1	C	269	ASP	3.2
1	A	401	THR	3.2
1	A	43	MET	3.1
1	A	618	PHE	3.0
1	C	459	VAL	3.0
1	C	341	ASN	3.0
1	C	460	GLN	2.9
1	A	45	ILE	2.7
1	C	186	ASP	2.7
1	A	341	ASN	2.7
1	A	186	ASP	2.7
1	B	186	ASP	2.7
1	B	618	PHE	2.7
1	C	309	PHE	2.6
1	C	307	ASP	2.6
1	C	561	GLU	2.6
1	D	272	GLU	2.6
1	D	391	TYR	2.6
1	D	387	GLY	2.6
1	A	389	LEU	2.5
1	B	340	PRO	2.5
1	A	460	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	392	SER	2.4
1	D	418	GLN	2.4
1	A	386	PRO	2.4
1	B	45	ILE	2.3
1	C	185	LYS	2.3
1	D	459	VAL	2.2
1	A	390	THR	2.2
1	D	189	ASP	2.2
1	C	617	PRO	2.2
1	C	388	GLU	2.2
1	D	188	ALA	2.1
1	A	309	PHE	2.1
1	C	190	ALA	2.1
1	C	272	GLU	2.1
1	C	187	ASP	2.1
1	A	347	GLU	2.1
1	B	389	LEU	2.0
1	D	381	THR	2.0
1	B	82	SER	2.0
1	B	617	PRO	2.0
1	C	189	ASP	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	FAD	D	5551	53/53	0.56	0.54	27.27	5,8,10,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FAD	C	6661	53/53	0.60	0.65	24.84	6,9,12,15	0
2	ACT	B	3901	4/4	0.92	0.14	7.30	15,16,18,19	0
4	12P	D	5002	19/37	0.64	0.21	6.06	55,59,67,67	0
4	12P	C	6002	13/37	0.67	0.23	5.74	67,71,75,76	0
4	12P	A	4002	19/37	0.70	0.25	4.10	66,74,80,80	0
4	12P	B	3102	12/37	0.75	0.19	3.75	59,63,65,66	0
4	12P	B	3105	10/37	0.89	0.17	2.95	50,54,62,66	0
2	ACT	C	6901	4/4	0.89	0.15	2.28	18,20,21,22	0
4	12P	B	3103	11/37	0.67	0.19	1.95	53,63,67,67	0
4	12P	A	5001	16/37	0.90	0.12	1.46	25,34,53,56	0
4	12P	D	5005	19/37	0.91	0.15	1.29	35,41,54,56	0
4	12P	A	4003	11/37	0.77	0.16	1.13	52,61,68,69	0
4	12P	B	3101	16/37	0.91	0.12	1.08	27,32,59,65	0
4	12P	C	6003	11/37	0.68	0.18	1.02	52,60,69,72	0
4	12P	B	6001	16/37	0.90	0.12	0.91	31,38,63,68	0
4	12P	D	5003	11/37	0.78	0.18	0.82	50,58,72,72	0
4	12P	C	6005	14/37	0.87	0.13	0.40	41,47,60,62	0
2	ACT	A	4901	4/4	0.97	0.10	0.25	16,17,17,21	0
4	12P	A	4001	12/37	0.94	0.08	-0.01	28,33,37,40	0
3	FAD	A	3331	53/53	0.98	0.10	-0.06	2,6,8,10	0
3	FAD	B	4441	53/53	0.98	0.09	-0.61	2,6,8,11	0
2	ACT	D	5901	4/4	0.95	0.08	-1.42	18,19,19,20	0
4	12P	A	4004	9/37	0.77	0.18	-	69,74,84,86	0
4	12P	C	6004	10/37	0.51	0.29	-	58,76,93,93	0
4	12P	D	5004	8/37	0.82	0.13	-	72,76,82,83	0
4	12P	B	3104	7/37	0.78	0.18	-	61,66,74,76	0
4	12P	D	4101	4/37	0.79	0.19	-	45,51,54,59	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.