



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:58 AM GMT

PDB ID : 4MOK  
Title : Pyranose 2-oxidase H167A mutant soaked with 3-fluorinated galactose (not bound)  
Authors : Tan, T.C.; Spadiut, O.; Gandini, R.; Haltrich, D.; Divne, C.  
Deposited on : 2013-09-12  
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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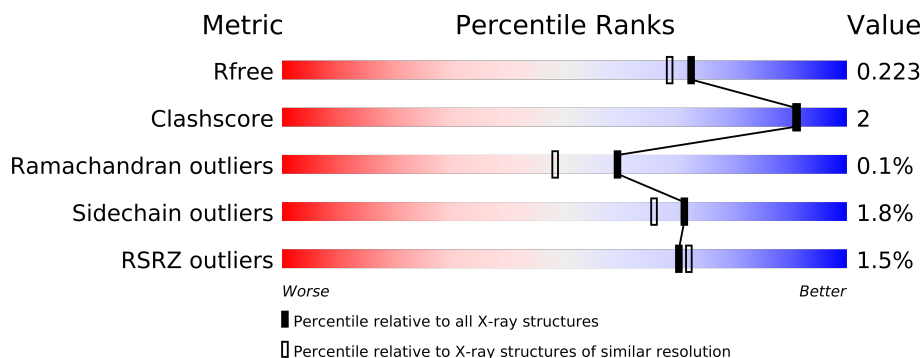
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.90 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))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	633	
1	B	633	
1	C	633	
1	D	633	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	12P	A	802	-	X
3	12P	B	802	-	X
3	12P	C	802	-	X
4	MES	A	803	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20179 atoms, of which 0 are hydrogen and 0 are deuterium.

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 2-oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4537	2865	775	872	25			
1	B	575	Total	C	N	O	S	0	0	0
			4529	2860	774	871	24			
1	C	574	Total	C	N	O	S	0	0	0
			4521	2856	773	868	24			
1	D	572	Total	C	N	O	S	0	0	0
			4502	2841	771	866	24			

There are 52 discrepancies between the modelled and reference sequences:

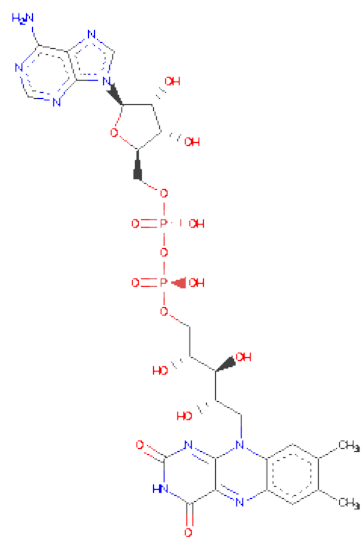
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
A	167	ALA	HIS	ENGINEERED MUTATION	UNP Q7ZA32
A	623	ALA	-	EXPRESSION TAG	UNP Q7ZA32
A	624	ALA	-	EXPRESSION TAG	UNP Q7ZA32
A	625	ALA	-	EXPRESSION TAG	UNP Q7ZA32
A	626	LEU	-	EXPRESSION TAG	UNP Q7ZA32
A	627	GLU	-	EXPRESSION TAG	UNP Q7ZA32
A	628	HIS	-	EXPRESSION TAG	UNP Q7ZA32
A	629	HIS	-	EXPRESSION TAG	UNP Q7ZA32
A	630	HIS	-	EXPRESSION TAG	UNP Q7ZA32
A	631	HIS	-	EXPRESSION TAG	UNP Q7ZA32
A	632	HIS	-	EXPRESSION TAG	UNP Q7ZA32
A	633	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
B	167	ALA	HIS	ENGINEERED MUTATION	UNP Q7ZA32
B	623	ALA	-	EXPRESSION TAG	UNP Q7ZA32
B	624	ALA	-	EXPRESSION TAG	UNP Q7ZA32
B	625	ALA	-	EXPRESSION TAG	UNP Q7ZA32
B	626	LEU	-	EXPRESSION TAG	UNP Q7ZA32
B	627	GLU	-	EXPRESSION TAG	UNP Q7ZA32
B	628	HIS	-	EXPRESSION TAG	UNP Q7ZA32

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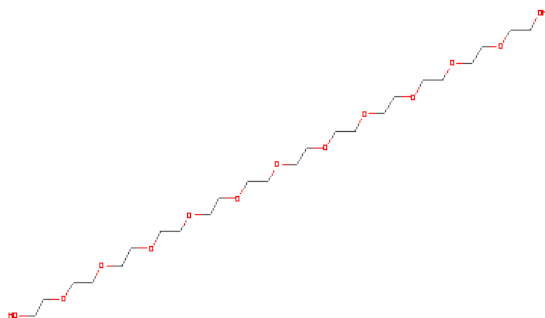
Chain	Residue	Modelled	Actual	Comment	Reference
B	629	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	630	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	631	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	632	HIS	-	EXPRESSION TAG	UNP Q7ZA32
B	633	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
C	167	ALA	HIS	ENGINEERED MUTATION	UNP Q7ZA32
C	623	ALA	-	EXPRESSION TAG	UNP Q7ZA32
C	624	ALA	-	EXPRESSION TAG	UNP Q7ZA32
C	625	ALA	-	EXPRESSION TAG	UNP Q7ZA32
C	626	LEU	-	EXPRESSION TAG	UNP Q7ZA32
C	627	GLU	-	EXPRESSION TAG	UNP Q7ZA32
C	628	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	629	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	630	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	631	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	632	HIS	-	EXPRESSION TAG	UNP Q7ZA32
C	633	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
D	167	ALA	HIS	ENGINEERED MUTATION	UNP Q7ZA32
D	623	ALA	-	EXPRESSION TAG	UNP Q7ZA32
D	624	ALA	-	EXPRESSION TAG	UNP Q7ZA32
D	625	ALA	-	EXPRESSION TAG	UNP Q7ZA32
D	626	LEU	-	EXPRESSION TAG	UNP Q7ZA32
D	627	GLU	-	EXPRESSION TAG	UNP Q7ZA32
D	628	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	629	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	630	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	631	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	632	HIS	-	EXPRESSION TAG	UNP Q7ZA32
D	633	HIS	-	EXPRESSION TAG	UNP Q7ZA32

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



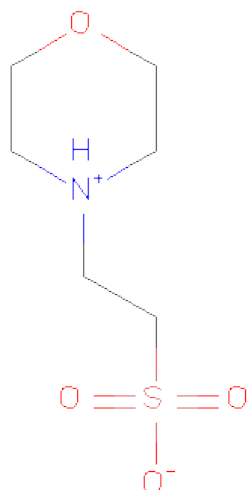
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is DODECAETHYLENE GLYCOL (three-letter code: 12P) (formula: C<sub>24</sub>H<sub>50</sub>O<sub>13</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			16	10	6		
3	C	1	Total	C	O	0	0
			16	10	6		
3	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	536	Total	O	0	0
			536	536		
5	B	498	Total	O	0	0
			498	498		
5	C	449	Total	O	0	0
			449	449		

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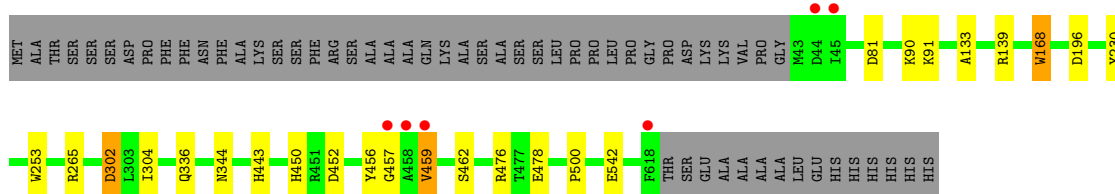
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	310	Total 310	O 310	0	0

### 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.

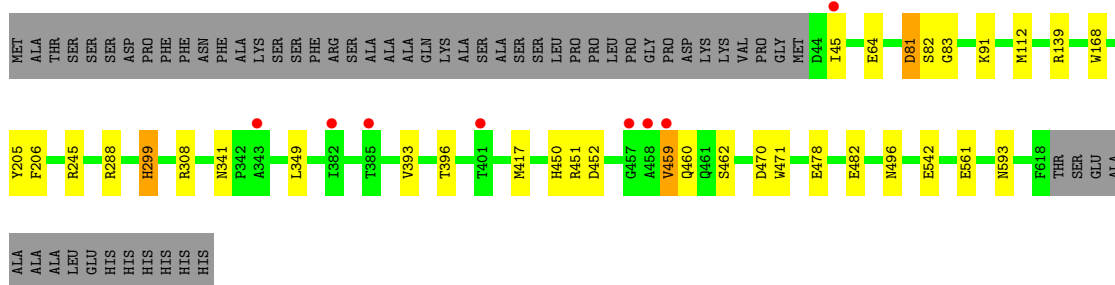
- Molecule 1: Pyranose 2-oxidase

Chain A: 



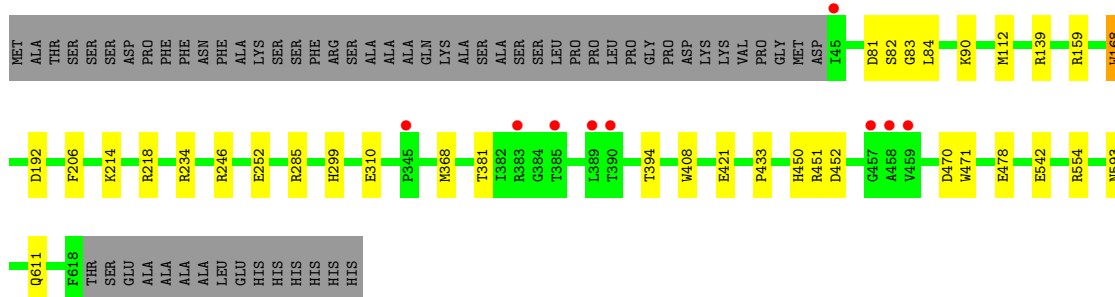
- Molecule 1: Pyranose 2-oxidase

Chain B: 



- Molecule 1: Pyranose 2-oxidase

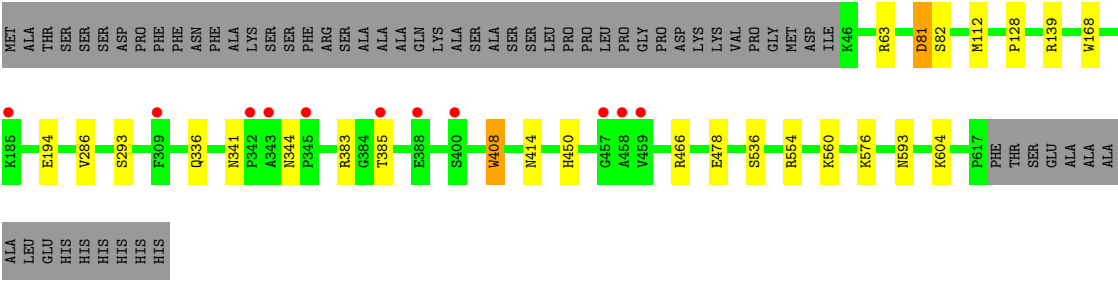
Chain C: 



- Molecule 1: Pyranose 2-oxidase

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.88Å 102.30Å 136.96Å 90.00° 90.78° 90.00°	Depositor
Resolution (Å)	47.92 – 1.90 45.65 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.92-1.90) 99.8 (45.65-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.170 , 0.214 0.178 , 0.223	Depositor DCC
$R_{free}$ test set	1066 reflections (0.50%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.3	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 35.1	EDS
Estimated twinning fraction	0.011 for -k,-h,-l 0.008 for k,h,-l 0.018 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 216233 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	20179	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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, MES

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	1.06	7/4652 (0.2%)	0.97	7/6325 (0.1%)
1	B	1.02	5/4644 (0.1%)	0.95	8/6315 (0.1%)
1	C	0.95	4/4636 (0.1%)	0.93	9/6304 (0.1%)
1	D	0.85	3/4616 (0.1%)	0.86	7/6277 (0.1%)
All	All	0.97	19/18548 (0.1%)	0.93	31/25221 (0.1%)

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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	478	GLU	CD-OE1	7.62	1.34	1.25
1	A	253	TRP	CD2-CE2	7.27	1.50	1.41
1	A	478	GLU	CD-OE1	7.00	1.33	1.25
1	B	471	TRP	CD2-CE2	6.35	1.49	1.41
1	C	168	TRP	CD2-CE2	6.34	1.49	1.41
1	C	478	GLU	CD-OE1	5.96	1.32	1.25
1	B	542	GLU	CD-OE1	5.80	1.32	1.25
1	A	542	GLU	CD-OE2	5.75	1.31	1.25
1	A	443	HIS	CG-CD2	5.75	1.45	1.35
1	B	482	GLU	CD-OE1	5.70	1.31	1.25
1	B	299	HIS	CG-CD2	5.69	1.45	1.35
1	D	408	TRP	CD2-CE2	5.62	1.48	1.41
1	D	536	SER	CB-OG	-5.56	1.35	1.42
1	C	542	GLU	CD-OE1	5.51	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	542	GLU	CD-OE1	5.40	1.31	1.25
1	D	478	GLU	CD-OE1	5.29	1.31	1.25
1	A	456	TYR	CE1-CZ	-5.26	1.31	1.38
1	C	471	TRP	CD2-CE2	5.26	1.47	1.41
1	A	168	TRP	CD2-CE2	5.19	1.47	1.41

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ARG	NE-CZ-NH2	-11.52	114.54	120.30
1	A	139	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	D	139	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	D	466	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	B	139	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	B	451	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	A	302	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	C	139	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	B	245	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	B	139	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	D	383	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	C	554	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	C	452	ASP	CB-CG-OD2	6.19	123.87	118.30
1	C	192	ASP	CB-CG-OD1	6.18	123.87	118.30
1	D	81	ASP	CB-CG-OD1	-6.18	112.74	118.30
1	A	302	ASP	CB-CG-OD1	6.04	123.74	118.30
1	B	288	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	C	470	ASP	CB-CG-OD1	5.79	123.51	118.30
1	C	368	MET	CG-SD-CE	5.74	109.39	100.20
1	B	349	LEU	CB-CG-CD2	5.73	120.74	111.00
1	C	218	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	D	383	ARG	CG-CD-NE	5.51	123.38	111.80
1	B	470	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	C	234	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	476	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	D	81	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	265	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	D	63	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	196	ASP	CB-CG-OD1	5.09	122.89	118.30
1	C	159	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	81	ASP	CB-CG-OD1	-5.04	113.76	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	230	TYR	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4537	0	0	9	0
1	B	4529	0	0	11	0
1	C	4521	0	0	9	0
1	D	4502	0	0	9	0
2	A	53	0	31	0	0
2	B	53	0	30	0	0
2	C	53	0	30	0	0
2	D	53	0	29	0	0
3	A	16	0	21	0	0
3	B	16	0	21	0	0
3	C	16	0	21	0	0
3	D	13	0	16	0	0
4	A	12	0	13	2	0
4	C	12	0	13	0	0
5	A	536	0	0	1	0
5	B	498	0	0	6	0
5	C	449	0	0	2	0
5	D	310	0	0	1	0
All	All	20179	0	225	38	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (38) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:133:ALA:CB	4:A:803:MES:H71	2.03	0.89
1:B:417:MET:SD	5:B:1356:HOH:O	2.38	0.81
1:B:308:ARG:NH1	5:B:1383:HOH:O	2.24	0.69
1:A:81:ASP:OD2	1:A:90:LYS:NZ	2.27	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:81:ASP:C	1:D:81:ASP:OD1	2.32	0.63
1:C:81:ASP:OD2	1:C:90:LYS:NZ	2.31	0.63
1:B:81:ASP:O	1:B:83:GLY:N	2.37	0.58
1:A:133:ALA:CB	4:A:803:MES:O1S	2.52	0.57
1:B:81:ASP:N	1:B:81:ASP:OD1	2.36	0.55
1:C:81:ASP:N	1:C:81:ASP:OD1	2.38	0.53
1:C:299:HIS:NE2	1:C:310:GLU:CG	2.72	0.52
1:D:293:SER:O	1:D:576:LYS:NZ	2.43	0.52
1:A:81:ASP:CG	1:A:90:LYS:NZ	2.64	0.51
1:B:393:VAL:CG2	5:B:1356:HOH:O	2.58	0.51
1:D:81:ASP:CG	1:D:81:ASP:O	2.47	0.50
1:D:81:ASP:N	1:D:81:ASP:OD1	2.43	0.48
1:B:299:HIS:CG	5:B:1374:HOH:O	2.66	0.48
1:A:459:VAL:CG1	1:A:459:VAL:O	2.62	0.48
1:B:91:LYS:NZ	1:B:452:ASP:OD1	2.47	0.48
1:B:459:VAL:CG1	1:B:460:GLN:N	2.78	0.47
1:C:84:LEU:N	5:C:1200:HOH:O	2.48	0.46
1:C:81:ASP:O	1:C:83:GLY:N	2.49	0.46
1:A:91:LYS:NZ	1:A:452:ASP:OD1	2.49	0.46
1:D:194:GLU:OE2	1:D:604:LYS:NZ	2.48	0.46
1:D:414:ASN:ND2	5:D:1068:HOH:O	2.48	0.46
1:B:393:VAL:N	5:B:1356:HOH:O	2.50	0.45
1:C:246:ARG:NH2	1:C:252:GLU:OE1	2.51	0.44
1:B:64:GLU:OE2	1:B:205:TYR:OH	2.35	0.43
1:D:336:GLN:OE1	1:D:341:ASN:N	2.51	0.43
1:D:81:ASP:OD1	1:D:81:ASP:O	2.37	0.42
1:A:336:GLN:NE2	1:A:344:ASN:O	2.53	0.42
1:D:341:ASN:ND2	1:D:344:ASN:ND2	2.67	0.42
1:A:302:ASP:OD1	1:A:304:ILE:N	2.53	0.42
1:B:396:THR:N	5:B:1193:HOH:O	2.52	0.41
1:C:451:ARG:NE	5:C:1127:HOH:O	2.53	0.41
1:C:421:GLU:N	1:C:421:GLU:OE1	2.53	0.41
1:A:457:GLY:CA	5:A:1235:HOH:O	2.69	0.41
1:C:381:THR:N	1:C:394:THR:O	2.55	0.40

There are no symmetry-related clashes.

## 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	574/633 (91%)	562 (98%)	12 (2%)	0	100	100
1	B	573/633 (90%)	553 (96%)	18 (3%)	2 (0%)	50	37
1	C	572/633 (90%)	550 (96%)	21 (4%)	1 (0%)	56	44
1	D	570/633 (90%)	549 (96%)	21 (4%)	0	100	100
All	All	2289/2532 (90%)	2214 (97%)	72 (3%)	3 (0%)	59	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	82	SER
1	C	82	SER
1	B	459	VAL

### 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	503/547 (92%)	498 (99%)	5 (1%)	85	84
1	B	502/547 (92%)	492 (98%)	10 (2%)	68	61
1	C	501/547 (92%)	491 (98%)	10 (2%)	68	61
1	D	499/547 (91%)	488 (98%)	11 (2%)	64	57
All	All	2005/2188 (92%)	1969 (98%)	36 (2%)	71	66

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	TRP
1	A	450	HIS
1	A	459	VAL
1	A	462	SER
1	A	500	PRO
1	B	45	ILE
1	B	112	MET
1	B	168	TRP
1	B	206	PHE
1	B	341	ASN
1	B	450	HIS
1	B	462	SER
1	B	496	ASN
1	B	561	GLU
1	B	593	ASN
1	C	112	MET
1	C	168	TRP
1	C	206	PHE
1	C	214	LYS
1	C	285	ARG
1	C	408	TRP
1	C	433	PRO
1	C	450	HIS
1	C	593	ASN
1	C	611	GLN
1	D	82	SER
1	D	112	MET
1	D	128	PRO
1	D	168	TRP
1	D	286	VAL
1	D	385	THR
1	D	408	TRP
1	D	450	HIS
1	D	554	ARG
1	D	560	LYS
1	D	593	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

10 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	801	-	58,58,58	1.47	7 (12%)	85,89,89	2.52	23 (27%)
3	12P	A	802	-	15,15,36	0.77	0	14,14,35	0.49	0
4	MES	A	803	-	12,12,12	1.69	1 (8%)	16,16,16	1.64	5 (31%)
2	FAD	B	801	-	58,58,58	1.46	7 (12%)	85,89,89	2.42	22 (25%)
3	12P	B	802	-	15,15,36	0.68	0	14,14,35	0.97	1 (7%)
2	FAD	C	801	-	58,58,58	1.49	7 (12%)	85,89,89	2.47	25 (29%)
3	12P	C	802	-	15,15,36	0.61	0	14,14,35	0.69	0
4	MES	C	803	-	12,12,12	1.75	1 (8%)	16,16,16	1.75	4 (25%)
2	FAD	D	801	-	58,58,58	1.43	7 (12%)	85,89,89	2.65	30 (35%)
3	12P	D	802	-	12,12,36	0.75	0	11,11,35	0.66	0

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	801	-	-	0/34/50/50	0/1/6/6
3	12P	A	802	-	-	0/13/13/34	0/0/0/0
4	MES	A	803	-	-	0/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	801	-	-	0/34/50/50	0/1/6/6
3	12P	B	802	-	-	0/13/13/34	0/0/0/0
2	FAD	C	801	-	-	0/34/50/50	0/1/6/6
3	12P	C	802	-	-	0/13/13/34	0/0/0/0
4	MES	C	803	-	-	0/6/14/14	0/1/1/1
2	FAD	D	801	-	-	0/34/50/50	0/1/6/6
3	12P	D	802	-	-	0/10/10/34	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	803	MES	C8-S	-5.48	1.68	1.78
2	D	801	FAD	C4-C4X	5.10	1.49	1.41
2	A	801	FAD	C6-C5X	4.95	1.47	1.41
2	B	801	FAD	C4-C4X	4.92	1.49	1.41
2	C	801	FAD	C4-C4X	4.80	1.49	1.41
4	A	803	MES	C8-S	-4.74	1.69	1.78
2	C	801	FAD	C2B-C1B	-4.22	1.47	1.53
2	C	801	FAD	C1'-C2'	4.22	1.55	1.51
2	A	801	FAD	C4-C4X	4.14	1.48	1.41
2	B	801	FAD	C4A-N9A	-3.44	1.32	1.37
2	A	801	FAD	C1'-C2'	3.42	1.54	1.51
2	D	801	FAD	P-O3P	3.19	1.65	1.59
2	B	801	FAD	C1'-N10	3.12	1.51	1.48
2	B	801	FAD	O4B-C4B	-2.99	1.38	1.45
2	D	801	FAD	C5'-C4'	2.97	1.56	1.51
2	D	801	FAD	O4B-C4B	-2.74	1.38	1.45
2	D	801	FAD	C2A-N1A	2.66	1.39	1.33
2	C	801	FAD	C4'-C3'	2.54	1.58	1.53
2	C	801	FAD	C2A-N1A	2.53	1.38	1.33
2	B	801	FAD	C2B-C1B	-2.44	1.50	1.53
2	B	801	FAD	O3B-C3B	-2.42	1.37	1.43
2	A	801	FAD	C2-N3	-2.36	1.32	1.37
2	A	801	FAD	C2B-C1B	-2.34	1.50	1.53
2	A	801	FAD	O4B-C1B	-2.30	1.37	1.41
2	A	801	FAD	O3B-C3B	-2.19	1.37	1.43
2	C	801	FAD	C2'-C3'	-2.12	1.49	1.53
2	B	801	FAD	O4B-C1B	2.09	1.44	1.41
2	D	801	FAD	O3B-C3B	-2.07	1.38	1.43
2	C	801	FAD	C2A-N3A	2.01	1.36	1.32
2	D	801	FAD	C4X-N5	-2.01	1.31	1.36

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	O4B-C1B-N9A	10.93	118.61	108.44
2	B	801	FAD	N3A-C2A-N1A	-10.19	120.19	128.71
2	A	801	FAD	C8A-N9A-C4A	9.66	114.27	106.90
2	D	801	FAD	N3A-C2A-N1A	-9.24	120.98	128.71
2	A	801	FAD	N3A-C2A-N1A	-9.17	121.05	128.71
2	C	801	FAD	N3A-C2A-N1A	-8.88	121.29	128.71
2	A	801	FAD	C2-N1-C10	8.54	123.59	114.98
2	C	801	FAD	C8A-N9A-C4A	8.44	113.34	106.90
2	B	801	FAD	C8A-N9A-C4A	8.44	113.34	106.90
2	D	801	FAD	C8A-N9A-C4A	8.05	113.04	106.90
2	B	801	FAD	C2-N1-C10	6.41	121.44	114.98
2	C	801	FAD	C4X-C10-N10	-6.23	117.40	120.51
2	C	801	FAD	O4B-C1B-N9A	5.78	113.82	108.44
2	D	801	FAD	C2-N1-C10	5.52	120.54	114.98
2	C	801	FAD	C2B-C1B-N9A	5.22	126.66	113.27
2	C	801	FAD	O3B-C3B-C4B	5.13	126.18	111.08
2	A	801	FAD	C4-N3-C2	5.00	135.66	125.39
2	D	801	FAD	C2B-C1B-N9A	4.94	125.94	113.27
2	B	801	FAD	C2B-C1B-N9A	4.85	125.71	113.27
2	B	801	FAD	C1'-N10-C9A	4.74	123.48	118.87
2	D	801	FAD	N3-C2-N1	-4.55	111.52	121.19
2	B	801	FAD	N3A-C4A-N9A	4.54	133.63	125.43
2	A	801	FAD	N3-C2-N1	-4.54	111.54	121.19
2	A	801	FAD	C2B-C1B-N9A	4.52	124.88	113.27
2	C	801	FAD	C2-N1-C10	4.37	119.38	114.98
2	B	801	FAD	O4B-C1B-N9A	4.34	112.47	108.44
2	C	801	FAD	N3A-C4A-N9A	4.22	133.04	125.43
2	C	801	FAD	O2B-C2B-C1B	4.14	123.74	111.23
2	A	801	FAD	N3A-C4A-N9A	4.05	132.74	125.43
2	A	801	FAD	O2B-C2B-C3B	3.98	124.77	111.83
2	D	801	FAD	O2B-C2B-C1B	3.96	123.20	111.23
2	B	801	FAD	C9A-N10-C10	-3.93	117.91	121.77
2	D	801	FAD	N3A-C4A-N9A	3.86	132.39	125.43
2	D	801	FAD	O3B-C3B-C4B	3.85	122.43	111.08
2	C	801	FAD	C4X-N5-C5X	3.78	120.93	116.69
2	B	801	FAD	C4-N3-C2	3.76	133.12	125.39
2	C	801	FAD	C4X-C10-N1	-3.63	119.11	122.73
4	A	803	MES	O2S-S-O1S	-3.55	105.59	112.44
2	C	801	FAD	C1'-N10-C9A	3.49	122.27	118.87
2	B	801	FAD	N3-C2-N1	-3.47	113.80	121.19
2	D	801	FAD	C4X-C10-N10	-3.48	118.78	120.51
2	A	801	FAD	C8A-N9A-C1B	-3.44	119.61	126.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FAD	N7A-C8A-N9A	-3.42	104.67	114.36
2	D	801	FAD	O2B-C2B-C3B	3.42	122.97	111.83
2	A	801	FAD	O4B-C4B-C3B	3.38	112.02	105.17
2	C	801	FAD	O2B-C2B-C3B	3.37	122.80	111.83
4	C	803	MES	C6-C5-N4	3.36	114.27	109.96
2	A	801	FAD	O4B-C1B-N9A	3.34	111.54	108.44
2	B	801	FAD	O2B-C2B-C1B	3.29	121.19	111.23
2	A	801	FAD	C3B-C2B-C1B	3.29	106.05	100.91
2	B	801	FAD	C8A-N9A-C1B	-3.27	119.93	126.38
2	A	801	FAD	N7A-C8A-N9A	-3.26	105.14	114.36
2	B	801	FAD	O2B-C2B-C3B	3.23	122.35	111.83
2	B	801	FAD	C4X-N5-C5X	3.20	120.28	116.69
2	A	801	FAD	C4X-C10-N10	-3.19	118.92	120.51
2	D	801	FAD	C4B-O4B-C1B	-3.12	106.36	109.75
2	B	801	FAD	C5B-C4B-C3B	3.05	127.43	115.21
2	A	801	FAD	C9A-N10-C10	-3.04	118.78	121.77
2	C	801	FAD	C5B-C4B-C3B	3.03	127.35	115.21
2	D	801	FAD	O4B-C4B-C5B	3.03	120.17	109.36
4	C	803	MES	O1-C2-C3	3.00	114.92	111.34
2	A	801	FAD	C5X-C9A-N10	2.98	119.73	116.80
4	C	803	MES	O2S-S-O1S	-2.97	106.70	112.44
2	D	801	FAD	C4X-C10-N1	-2.95	119.78	122.73
2	B	801	FAD	C9A-C5X-N5	-2.91	117.91	122.37
2	D	801	FAD	C2A-N1A-C6A	2.90	124.01	118.77
2	D	801	FAD	O4B-C1B-C2B	2.89	111.20	106.77
2	B	801	FAD	N7A-C8A-N9A	-2.88	106.22	114.36
2	B	801	FAD	C3B-C2B-C1B	2.81	105.31	100.91
2	D	801	FAD	N7A-C8A-N9A	-2.76	106.56	114.36
2	C	801	FAD	N3-C2-N1	-2.70	115.45	121.19
2	A	801	FAD	C4X-C4-N3	-2.70	107.50	115.39
2	D	801	FAD	C1'-N10-C9A	2.66	121.46	118.87
2	B	801	FAD	O4B-C4B-C5B	2.61	118.68	109.36
2	A	801	FAD	C5A-C4A-N9A	-2.60	103.41	107.16
2	D	801	FAD	O2A-PA-O1A	2.57	126.58	112.21
2	A	801	FAD	C4X-C10-N1	-2.55	120.18	122.73
2	D	801	FAD	C5B-C4B-C3B	2.55	125.43	115.21
4	A	803	MES	O3S-S-O1S	-2.49	106.08	112.48
2	A	801	FAD	C4X-N5-C5X	2.47	119.47	116.69
2	A	801	FAD	C2A-N1A-C6A	2.46	123.21	118.77
2	C	801	FAD	C2A-N1A-C6A	2.45	123.20	118.77
4	A	803	MES	C2-C3-N4	2.45	113.10	109.96
2	D	801	FAD	C9A-N10-C10	-2.42	119.39	121.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FAD	O4B-C4B-C5B	2.40	117.92	109.36
2	C	801	FAD	O4B-C1B-C2B	2.40	110.45	106.77
2	D	801	FAD	C5A-C4A-N9A	-2.36	103.76	107.16
2	C	801	FAD	C2'-C1'-N10	-2.33	109.36	112.45
2	C	801	FAD	O2A-PA-O1A	2.31	125.09	112.21
2	D	801	FAD	C8A-N9A-C1B	-2.29	121.86	126.38
2	A	801	FAD	O2B-C2B-C1B	2.27	118.10	111.23
2	D	801	FAD	C4-N3-C2	2.25	130.01	125.39
2	D	801	FAD	O4B-C4B-C3B	2.23	109.69	105.17
2	C	801	FAD	O2A-PA-O3P	2.23	115.72	105.14
2	B	801	FAD	O3B-C3B-C4B	2.22	117.61	111.08
4	C	803	MES	O3S-S-O2S	-2.20	106.83	112.48
2	C	801	FAD	O2'-C2'-C1'	-2.17	104.33	109.71
4	A	803	MES	O1-C2-C3	-2.15	108.78	111.34
2	B	801	FAD	C5A-C4A-N9A	-2.13	104.08	107.16
4	A	803	MES	O2S-S-C8	2.13	112.92	106.36
2	B	801	FAD	P-O3P-PA	2.12	137.90	131.68
2	C	801	FAD	C5A-C4A-N9A	-2.12	104.11	107.16
3	B	802	12P	C12-O13-C14	2.12	122.69	113.38
2	A	801	FAD	C1'-N10-C9A	2.07	120.88	118.87
2	D	801	FAD	O2A-PA-O3P	2.05	114.86	105.14
2	D	801	FAD	C9A-C5X-N5	-2.05	119.22	122.37
2	D	801	FAD	O3'-C3'-C4'	2.04	113.90	108.74
2	C	801	FAD	C8A-N7A-C5A	2.04	109.90	103.58
2	D	801	FAD	C4X-N5-C5X	2.02	118.96	116.69
2	D	801	FAD	O5'-P-O1P	-2.00	101.52	109.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	576/633 (90%)	-0.31	6 (1%) 79 81	17, 23, 45, 83	0
1	B	575/633 (90%)	-0.25	8 (1%) 72 74	18, 25, 51, 90	0
1	C	574/633 (90%)	-0.25	9 (1%) 68 70	19, 29, 53, 89	0
1	D	572/633 (90%)	-0.06	11 (1%) 64 65	22, 39, 65, 97	0
All	All	2297/2532 (90%)	-0.21	34 (1%) 70 72	17, 29, 58, 97	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	458	ALA	11.7
1	D	458	ALA	8.8
1	C	457	GLY	7.3
1	D	457	GLY	6.0
1	B	459	VAL	5.4
1	A	459	VAL	5.0
1	A	458	ALA	4.9
1	A	45	ILE	4.3
1	C	458	ALA	4.2
1	D	343	ALA	3.7
1	A	457	GLY	3.4
1	C	45	ILE	3.3
1	D	459	VAL	3.3
1	B	45	ILE	3.2
1	B	457	GLY	3.2
1	C	390	THR	3.1
1	D	385	THR	3.0
1	C	385	THR	2.8
1	D	185	LYS	2.7
1	D	388	GLU	2.6
1	C	389	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	345	PRO	2.6
1	C	383	ARG	2.6
1	D	400	SER	2.5
1	B	343	ALA	2.5
1	C	459	VAL	2.5
1	B	382	ILE	2.4
1	B	401	THR	2.3
1	D	309	PHE	2.3
1	D	342	PRO	2.3
1	D	345	PRO	2.2
1	A	44	ASP	2.1
1	B	385	THR	2.1
1	A	618	PHE	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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MES	A	803	12/12	0.20	4.83	45,58,60,62	0
3	12P	A	802	16/37	0.12	4.46	35,38,50,51	0
3	12P	C	802	16/37	0.12	3.50	28,36,52,55	0
3	12P	B	802	16/37	0.13	3.40	31,37,50,59	0
3	12P	D	802	13/37	0.12	1.12	39,41,51,57	0
4	MES	C	803	12/12	0.10	0.69	42,44,49,50	0
2	FAD	A	801	53/53	0.10	-0.43	14,18,21,22	0
2	FAD	C	801	53/53	0.10	-0.50	19,24,28,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	B	801	53/53	0.10	-0.51	16,19,23,24	0
2	FAD	D	801	53/53	0.09	-0.51	26,32,36,38	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.