



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:38 PM GMT

PDB ID : 4GDP  
Title : Yeast polyamine oxidase FMS1, N195A mutant  
Authors : Taylor, A.B.; Adachi, M.S.; Hart, P.J.; Fitzpatrick, P.F.  
Deposited on : 2012-08-01  
Resolution : 2.00 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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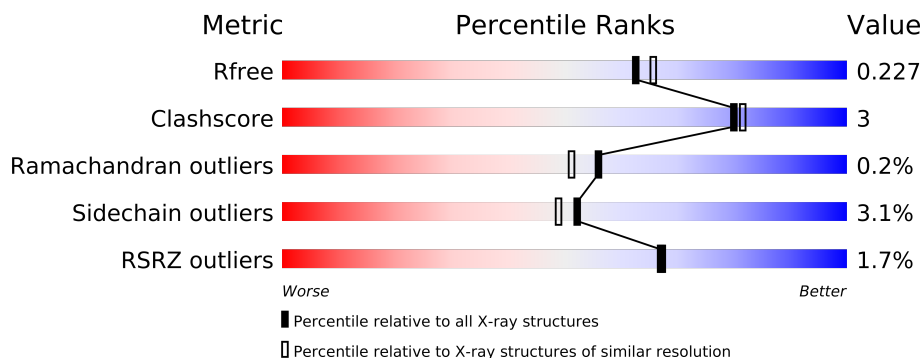
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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	516	
1	B	516	
1	C	516	
1	D	516	

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	PG4	D	802	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16892 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 Polyamine oxidase FMS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	2	0
			3967	2505	689	751	22			
1	B	502	Total	C	N	O	S	0	3	0
			4029	2544	698	763	24			
1	C	488	Total	C	N	O	S	0	1	0
			3916	2474	679	740	23			
1	D	498	Total	C	N	O	S	0	2	0
			3997	2525	693	757	22			

There are 36 discrepancies between the modelled and reference sequences:

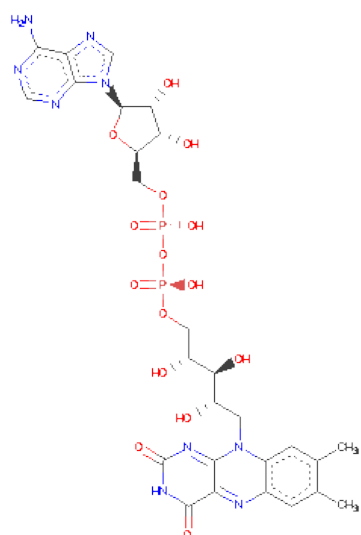
Chain	Residue	Modelled	Actual	Comment	Reference
A	195	ALA	ASN	ENGINEERED MUTATION	UNP P50264
A	509	LEU	-	EXPRESSION TAG	UNP P50264
A	510	GLU	-	EXPRESSION TAG	UNP P50264
A	511	HIS	-	EXPRESSION TAG	UNP P50264
A	512	HIS	-	EXPRESSION TAG	UNP P50264
A	513	HIS	-	EXPRESSION TAG	UNP P50264
A	514	HIS	-	EXPRESSION TAG	UNP P50264
A	515	HIS	-	EXPRESSION TAG	UNP P50264
A	516	HIS	-	EXPRESSION TAG	UNP P50264
B	195	ALA	ASN	ENGINEERED MUTATION	UNP P50264
B	509	LEU	-	EXPRESSION TAG	UNP P50264
B	510	GLU	-	EXPRESSION TAG	UNP P50264
B	511	HIS	-	EXPRESSION TAG	UNP P50264
B	512	HIS	-	EXPRESSION TAG	UNP P50264
B	513	HIS	-	EXPRESSION TAG	UNP P50264
B	514	HIS	-	EXPRESSION TAG	UNP P50264
B	515	HIS	-	EXPRESSION TAG	UNP P50264
B	516	HIS	-	EXPRESSION TAG	UNP P50264
C	195	ALA	ASN	ENGINEERED MUTATION	UNP P50264
C	509	LEU	-	EXPRESSION TAG	UNP P50264
C	510	GLU	-	EXPRESSION TAG	UNP P50264

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Chain	Residue	Modelled	Actual	Comment	Reference
C	511	HIS	-	EXPRESSION TAG	UNP P50264
C	512	HIS	-	EXPRESSION TAG	UNP P50264
C	513	HIS	-	EXPRESSION TAG	UNP P50264
C	514	HIS	-	EXPRESSION TAG	UNP P50264
C	515	HIS	-	EXPRESSION TAG	UNP P50264
C	516	HIS	-	EXPRESSION TAG	UNP P50264
D	195	ALA	ASN	ENGINEERED MUTATION	UNP P50264
D	509	LEU	-	EXPRESSION TAG	UNP P50264
D	510	GLU	-	EXPRESSION TAG	UNP P50264
D	511	HIS	-	EXPRESSION TAG	UNP P50264
D	512	HIS	-	EXPRESSION TAG	UNP P50264
D	513	HIS	-	EXPRESSION TAG	UNP P50264
D	514	HIS	-	EXPRESSION TAG	UNP P50264
D	515	HIS	-	EXPRESSION TAG	UNP P50264
D	516	HIS	-	EXPRESSION TAG	UNP P50264

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



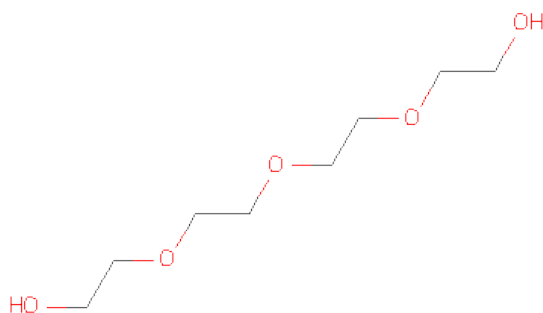
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0

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

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	B	1	Total	C	O	0	0
			11	7	4		
3	C	1	Total	C	O	0	0
			13	8	5		
3	D	1	Total	C	O	0	0
			11	8	3		

- Molecule 4 is water.

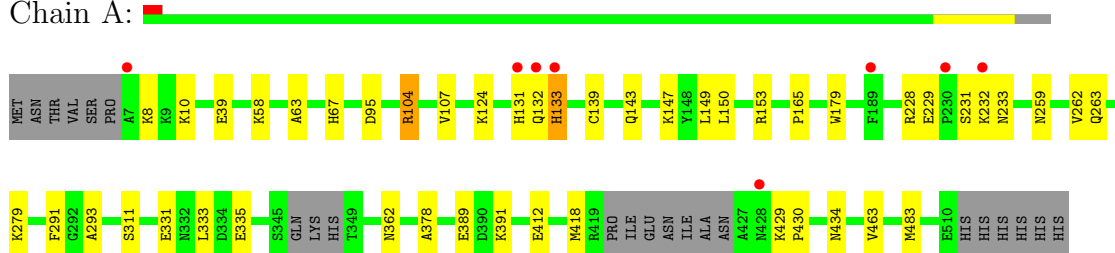
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	163	Total	O	0	0
			163	163		
4	B	199	Total	O	0	0
			199	199		
4	C	161	Total	O	0	0
			161	161		
4	D	200	Total	O	0	0
			200	200		

### 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.

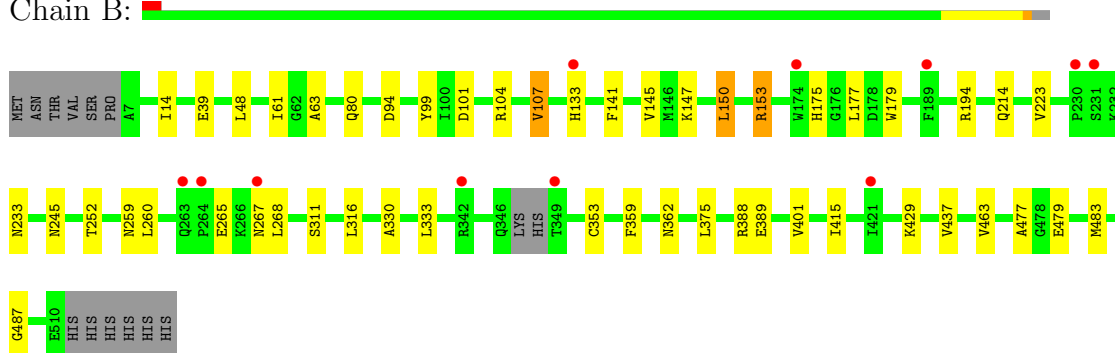
- Molecule 1: Polyamine oxidase FMS1

Chain A:



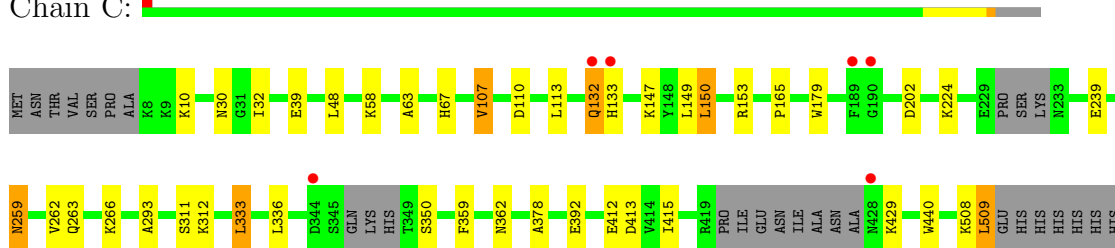
- Molecule 1: Polyamine oxidase FMS1

Chain B:



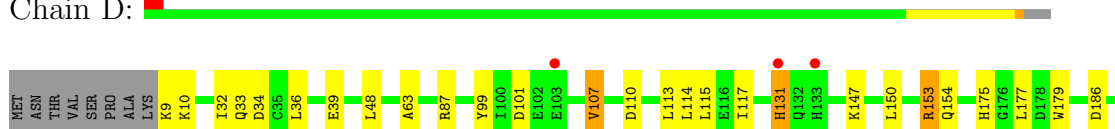
- Molecule 1: Polyamine oxidase FMS1

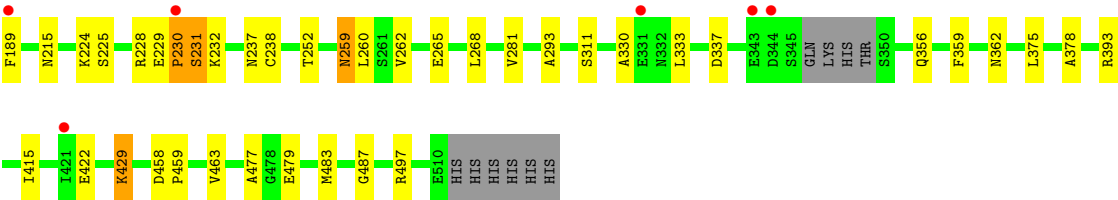
Chain C:



- Molecule 1: Polyamine oxidase FMS1

Chain D:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.85Å 81.89Å 104.79Å 78.07° 79.51° 78.92°	Depositor
Resolution (Å)	79.07 – 2.00 79.08 – 2.00	Depositor EDS
% Data completeness (in resolution range)	88.9 (79.07-2.00) 88.9 (79.08-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.203 , 0.234 0.196 , 0.227	Depositor DCC
$R_{free}$ test set	2004 reflections (1.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.5	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 28.5	EDS
Estimated twinning fraction	0.138 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 149579 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16892	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: PG4, 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	0.28	0/4050	0.44	0/5474
1	B	0.28	0/4119	0.44	0/5570
1	C	0.28	0/3996	0.43	0/5399
1	D	0.28	0/4084	0.44	0/5523
All	All	0.28	0/16249	0.44	0/21966

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3967	0	3885	23	0
1	B	4029	0	3955	26	0
1	C	3916	0	3837	24	0
1	D	3997	0	3921	38	0
2	A	53	0	31	4	0
2	B	53	0	31	2	0
2	C	53	0	31	2	0
2	D	53	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	13	0	18	2	0
3	B	11	0	13	0	0
3	C	13	0	18	2	0
3	D	11	0	12	0	0
4	A	163	0	0	2	0
4	B	199	0	0	3	0
4	C	161	0	0	1	0
4	D	200	0	0	4	0
All	All	16892	0	15783	110	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 3.

All (110) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:14:ILE:HD12	1:B:223:VAL:HG21	1.65	0.78
1:C:412:GLU:HG3	1:C:429:LYS:HE3	1.73	0.70
1:D:229:GLU:O	1:D:231:SER:N	2.22	0.70
1:D:9:LYS:N	1:D:34:ASP:O	2.26	0.68
1:A:133:HIS:O	1:D:393:ARG:NH2	2.29	0.65
1:C:67:HIS:HE1	3:C:802:PG4:H71	1.63	0.64
1:C:149:LEU:HD11	1:C:165:PRO:HG3	1.80	0.62
1:D:153:ARG:NH2	1:D:330:ALA:O	2.31	0.62
1:A:279:LYS:NZ	4:A:1048:HOH:O	2.34	0.61
1:C:150:LEU:HD23	1:C:336:LEU:HD22	1.84	0.60
1:C:10:LYS:HE2	1:C:32:ILE:HG23	1.83	0.59
1:A:149:LEU:HD11	1:A:165:PRO:HG3	1.85	0.58
1:C:39:GLU:OE1	2:C:801:FAD:O2B	2.22	0.58
1:B:80:GLN:NE2	4:B:1009:HOH:O	2.34	0.57
1:C:508:LYS:O	1:C:509:LEU:HB2	2.05	0.57
1:A:39:GLU:OE1	2:A:801:FAD:O2B	2.22	0.56
1:B:99:TYR:HB3	1:B:316:LEU:HD21	1.87	0.56
1:B:147:LYS:HG2	1:B:333:LEU:HD11	1.87	0.56
1:C:67:HIS:CE1	3:C:802:PG4:H71	2.40	0.55
1:D:293:ALA:HB3	1:D:378:ALA:HB2	1.89	0.55
1:C:415:ILE:HD11	1:C:429:LYS:HD3	1.90	0.54
1:A:311:SER:HA	1:A:362:ASN:HB3	1.89	0.54
1:A:10:LYS:NZ	4:A:1007:HOH:O	2.40	0.54
1:C:311:SER:HA	1:C:362:ASN:HB3	1.90	0.54
1:B:214:GLN:NE2	4:B:993:HOH:O	2.40	0.54
1:D:497:ARG:NE	4:D:1069:HOH:O	2.41	0.54
1:A:293:ALA:HB3	1:A:378:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:293:ALA:HB3	1:C:378:ALA:HB2	1.91	0.53
1:B:39:GLU:OE1	2:B:801:FAD:O2B	2.27	0.53
1:A:8:LYS:HE2	1:A:233:ASN:HD21	1.75	0.52
1:A:139:CYS:HB2	1:A:143:GLN:OE1	2.10	0.52
1:D:131:HIS:ND1	1:D:131:HIS:O	2.44	0.51
1:B:252:THR:HG22	1:B:477:ALA:HB3	1.92	0.51
1:D:147:LYS:HG2	1:D:333:LEU:HD11	1.93	0.50
1:D:39:GLU:OE1	2:D:801:FAD:O2B	2.29	0.49
1:D:224:LYS:NZ	1:D:238:CYS:O	2.45	0.49
1:B:359:PHE:HD2	1:B:375:LEU:HD22	1.77	0.49
1:C:147:LYS:HG2	1:C:333:LEU:HD21	1.95	0.49
1:B:48:LEU:HD23	1:B:63:ALA:HB3	1.95	0.49
1:D:479:GLU:OE1	1:D:487:GLY:HA2	2.13	0.48
1:D:359:PHE:HD2	1:D:375:LEU:HD22	1.78	0.48
1:B:353:CYS:SG	1:B:401:VAL:HG13	2.53	0.48
1:B:311:SER:HA	1:B:362:ASN:HB3	1.96	0.48
1:A:147:LYS:HD3	1:A:333:LEU:HD11	1.95	0.48
1:B:133:HIS:HD1	1:D:422:GLU:CD	2.17	0.48
1:D:110:ASP:HB3	1:D:113:LEU:HB2	1.95	0.47
1:C:132:GLN:HG3	1:C:133:HIS:CE1	2.49	0.47
1:D:186:ASP:HB2	4:D:1003:HOH:O	2.14	0.47
1:A:8:LYS:HE2	1:A:233:ASN:ND2	2.29	0.47
1:D:48:LEU:CD2	1:D:63:ALA:HB3	2.45	0.47
1:A:463:VAL:HG11	1:A:483:MET:HG2	1.97	0.47
1:A:67:HIS:HE1	3:A:802:PG4:H21	1.80	0.46
1:D:150:LEU:O	1:D:153:ARG:HD2	2.15	0.46
1:D:229:GLU:HA	1:D:230:PRO:HD3	1.82	0.46
1:D:463:VAL:HG11	1:D:483:MET:HG2	1.96	0.46
1:D:228:ARG:NE	1:D:232:LYS:O	2.35	0.46
1:B:48:LEU:CD2	1:B:63:ALA:HB3	2.46	0.46
1:C:58:LYS:NZ	1:C:202:ASP:OD2	2.48	0.45
1:A:228:ARG:HH21	1:A:232:LYS:HA	1.82	0.45
1:D:153:ARG:HG2	1:D:154:GLN:N	2.31	0.45
1:A:132:GLN:HB2	1:A:133:HIS:ND1	2.32	0.45
1:D:311:SER:HA	1:D:362:ASN:HB3	1.98	0.45
1:C:312:LYS:HD2	1:C:359:PHE:CZ	2.52	0.44
1:A:418:MET:HE3	1:A:434:ASN:HA	1.98	0.44
1:D:415:ILE:HD11	1:D:429:LYS:HD3	2.00	0.44
1:C:107:VAL:HG22	1:C:113:LEU:HD13	1.99	0.44
1:C:30:ASN:O	1:C:508:LYS:HE3	2.18	0.43
1:D:260:LEU:HD22	1:D:268:LEU:HD13	2.00	0.43
1:A:63:ALA:HA	2:A:801:FAD:C4X	2.48	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:415:ILE:HD11	1:B:429:LYS:HD3	2.00	0.43
1:C:48:LEU:HD22	1:C:63:ALA:HB3	2.00	0.43
1:D:114:LEU:HB3	1:D:117:ILE:HD12	1.99	0.43
1:B:153:ARG:NH2	1:B:330:ALA:O	2.45	0.43
1:D:215:ASN:ND2	4:D:1056:HOH:O	2.33	0.43
1:D:10:LYS:NZ	1:D:33:GLN:H	2.17	0.43
1:A:429:LYS:HA	1:A:430:PRO:HD3	1.89	0.43
1:C:63:ALA:HA	2:C:801:FAD:N5	2.34	0.43
1:D:281:VAL:HG22	4:D:1019:HOH:O	2.18	0.43
1:D:131:HIS:O	1:D:131:HIS:CG	2.72	0.43
1:A:412:GLU:HB3	1:A:429:LYS:HE3	2.01	0.42
1:A:63:ALA:HA	2:A:801:FAD:N5	2.34	0.42
1:D:359:PHE:CD2	1:D:375:LEU:HD22	2.54	0.42
1:C:224:LYS:HE3	1:C:239:GLU:HG2	2.02	0.42
1:D:107:VAL:HG13	1:D:115:LEU:HD12	2.01	0.42
1:D:225:SER:HB2	1:D:237:ASN:HB2	2.01	0.42
1:D:259:ASN:O	1:D:262:VAL:HG22	2.20	0.42
1:B:260:LEU:HD22	1:B:268:LEU:HD13	2.00	0.42
1:C:259:ASN:O	1:C:262:VAL:HG22	2.20	0.42
1:C:413:ASP:O	1:C:429:LYS:HE2	2.20	0.41
1:C:440:TRP:HB2	4:C:981:HOH:O	2.19	0.41
1:B:61:ILE:HA	1:B:61:ILE:HD12	1.88	0.41
1:A:147:LYS:HE2	1:A:147:LYS:HB2	1.60	0.41
1:D:10:LYS:HD2	1:D:32:ILE:HG23	2.03	0.41
1:B:141:PHE:O	1:B:145:VAL:HG23	2.20	0.41
1:A:104:ARG:O	1:A:104:ARG:HG3	2.21	0.41
1:B:94:ASP:OD1	1:B:194:ARG:HB3	2.20	0.41
1:B:104:ARG:HG2	1:B:107:VAL:HG23	2.03	0.41
1:B:487:GLY:O	2:B:801:FAD:O3'	2.38	0.41
1:B:150:LEU:HA	1:B:150:LEU:HD22	1.89	0.41
1:B:479:GLU:OE1	1:B:487:GLY:HA2	2.21	0.41
1:A:259:ASN:O	1:A:262:VAL:HG22	2.21	0.40
1:D:252:THR:HG22	1:D:477:ALA:HB3	2.03	0.40
1:B:463:VAL:HG11	1:B:483:MET:HG2	2.02	0.40
1:B:388:ARG:HB2	1:B:437:VAL:HB	2.04	0.40
2:A:801:FAD:N5	3:A:802:PG4:H51	2.36	0.40
1:D:99:TYR:HB2	1:D:107:VAL:HG12	2.04	0.40
1:D:458:ASP:HA	1:D:459:PRO:HD2	1.83	0.40
1:C:110:ASP:HB3	1:C:113:LEU:HB2	2.03	0.40
1:D:175:HIS:CE1	1:D:189:PHE:HE2	2.40	0.40
1:B:175:HIS:HD2	4:B:955:HOH:O	2.04	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	490/516 (95%)	473 (96%)	17 (4%)	0	100	100
1	B	501/516 (97%)	488 (97%)	13 (3%)	0	100	100
1	C	481/516 (93%)	464 (96%)	16 (3%)	1 (0%)	56	51
1	D	496/516 (96%)	480 (97%)	14 (3%)	2 (0%)	43	36
All	All	1968/2064 (95%)	1905 (97%)	60 (3%)	3 (0%)	56	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	132	GLN
1	D	231	SER
1	D	230	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	437/456 (96%)	419 (96%)	18 (4%)	41	35
1	B	445/456 (98%)	433 (97%)	12 (3%)	57	56
1	C	432/456 (95%)	421 (98%)	11 (2%)	60	59
1	D	441/456 (97%)	428 (97%)	13 (3%)	55	52
All	All	1755/1824 (96%)	1701 (97%)	54 (3%)	52	49

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	95	ASP
1	A	104	ARG
1	A	107	VAL
1	A	124	LYS
1	A	131	HIS
1	A	133	HIS
1	A	150	LEU
1	A	153	ARG
1	A	179	TRP
1	A	229	GLU
1	A	231	SER
1	A	263	GLN
1	A	291	PHE
1	A	331	GLU
1	A	335	GLU
1	A	389	GLU
1	A	391	LYS
1	B	101	ASP
1	B	107	VAL
1	B	150	LEU
1	B	153	ARG
1	B	177	LEU
1	B	179	TRP
1	B	233	ASN
1	B	245	ASN
1	B	259	ASN
1	B	265	GLU
1	B	267	ASN
1	B	389	GLU
1	C	107	VAL
1	C	150	LEU
1	C	153	ARG
1	C	179	TRP
1	C	259	ASN
1	C	263	GLN
1	C	266	LYS
1	C	333	LEU
1	C	350	SER
1	C	392	GLU
1	C	509	LEU
1	D	36	LEU
1	D	87	ARG

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Mol	Chain	Res	Type
1	D	101	ASP
1	D	107	VAL
1	D	131	HIS
1	D	153	ARG
1	D	177	LEU
1	D	179	TRP
1	D	259	ASN
1	D	265	GLU
1	D	337	ASP
1	D	356	GLN
1	D	429	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	233	ASN
1	A	245	ASN
1	B	191	HIS
1	C	67	HIS

### 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 ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	FAD	A	801	-	58,58,58	1.69	10 (17%)	85,89,89	2.02	16 (18%)
3	PG4	A	802	-	12,12,12	0.68	0	11,11,11	1.40	0
2	FAD	B	801	-	58,58,58	1.68	10 (17%)	85,89,89	2.03	16 (18%)
3	PG4	B	802	-	9,10,12	0.94	1 (11%)	8,9,11	1.30	0
2	FAD	C	801	-	58,58,58	1.70	11 (18%)	85,89,89	2.26	20 (23%)
3	PG4	C	802	-	12,12,12	0.66	0	11,11,11	1.39	0
2	FAD	D	801	-	58,58,58	1.69	10 (17%)	85,89,89	2.03	16 (18%)
3	PG4	D	802	-	10,10,12	6.00	2 (20%)	7,9,11	1.70	1 (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	801	-	-	0/34/50/50	0/1/6/6
3	PG4	A	802	-	-	0/10/10/10	0/0/0/0
2	FAD	B	801	-	-	0/34/50/50	0/1/6/6
3	PG4	B	802	-	-	0/8/8/10	0/0/0/0
2	FAD	C	801	-	-	0/34/50/50	0/1/6/6
3	PG4	C	802	-	-	0/10/10/10	0/0/0/0
2	FAD	D	801	-	-	0/34/50/50	0/1/6/6
3	PG4	D	802	-	-	0/8/8/10	0/0/0/0

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802	PG4	C1-C2	-13.57	1.49	1.55
3	D	802	PG4	C8-C7	-13.02	1.50	1.55
2	B	801	FAD	C8M-C8	-5.20	1.39	1.51
2	A	801	FAD	C7M-C7	-5.19	1.39	1.51
2	D	801	FAD	C7M-C7	-5.19	1.39	1.51
2	C	801	FAD	C7M-C7	-5.19	1.39	1.51
2	D	801	FAD	C8M-C8	-5.18	1.39	1.51
2	C	801	FAD	C8M-C8	-5.18	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	FAD	C7M-C7	-5.16	1.40	1.51
2	A	801	FAD	C8M-C8	-5.14	1.40	1.51
2	C	801	FAD	C2A-N3A	4.03	1.40	1.32
2	A	801	FAD	C2A-N3A	4.03	1.40	1.32
2	D	801	FAD	C2A-N3A	4.02	1.40	1.32
2	B	801	FAD	C2A-N3A	4.02	1.40	1.32
2	D	801	FAD	C2A-N1A	3.10	1.40	1.33
2	A	801	FAD	C2A-N1A	3.08	1.40	1.33
2	B	801	FAD	C2A-N1A	3.08	1.40	1.33
2	C	801	FAD	C2A-N1A	3.06	1.39	1.33
2	D	801	FAD	C4A-N9A	-2.99	1.33	1.37
2	B	801	FAD	C4A-N9A	-2.99	1.33	1.37
2	A	801	FAD	C5A-C4A	-2.99	1.33	1.40
2	B	801	FAD	C5A-C4A	-2.97	1.33	1.40
2	D	801	FAD	C5A-C4A	-2.97	1.33	1.40
2	C	801	FAD	C5A-C4A	-2.95	1.33	1.40
2	C	801	FAD	C4A-N9A	-2.91	1.33	1.37
2	A	801	FAD	C4A-N9A	-2.91	1.33	1.37
2	D	801	FAD	C10-N1	2.67	1.40	1.35
2	A	801	FAD	C10-N1	2.65	1.40	1.35
2	C	801	FAD	C10-N1	2.64	1.40	1.35
2	B	801	FAD	C10-N1	2.63	1.40	1.35
2	B	801	FAD	C9A-N10	-2.59	1.35	1.38
2	D	801	FAD	C9A-N10	-2.59	1.35	1.38
2	A	801	FAD	C9A-N10	-2.58	1.35	1.38
2	C	801	FAD	C9A-N10	-2.54	1.35	1.38
2	A	801	FAD	C8A-N9A	-2.24	1.33	1.36
2	D	801	FAD	C8A-N9A	-2.21	1.33	1.36
2	B	801	FAD	C8A-N9A	-2.21	1.33	1.36
2	C	801	FAD	C8A-N9A	-2.17	1.33	1.36
3	B	802	PG4	O2-C3	-2.07	1.37	1.46
2	C	801	FAD	C1'-C2'	2.02	1.53	1.51
2	D	801	FAD	C10-N10	-2.02	1.34	1.38
2	B	801	FAD	C10-N10	-2.01	1.34	1.38
2	A	801	FAD	C10-N10	-2.01	1.34	1.38
2	C	801	FAD	C10-N10	-2.00	1.34	1.38

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FAD	N3A-C2A-N1A	-12.69	118.10	128.71
2	D	801	FAD	N3A-C2A-N1A	-12.66	118.12	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FAD	N3A-C2A-N1A	-12.64	118.14	128.71
2	A	801	FAD	N3A-C2A-N1A	-12.60	118.18	128.71
2	C	801	FAD	O5B-PA-O1A	-5.25	88.80	109.37
2	C	801	FAD	C4B-O4B-C1B	-5.18	104.12	109.75
2	D	801	FAD	C4B-O4B-C1B	-5.00	104.32	109.75
2	B	801	FAD	C4B-O4B-C1B	-4.97	104.35	109.75
2	A	801	FAD	C4B-O4B-C1B	-4.94	104.38	109.75
2	B	801	FAD	C2-N1-C10	4.83	119.85	114.98
2	C	801	FAD	C2-N1-C10	4.78	119.80	114.98
2	D	801	FAD	C2-N1-C10	4.77	119.78	114.98
2	A	801	FAD	C2-N1-C10	4.74	119.75	114.98
2	C	801	FAD	O3P-PA-O5B	-4.59	82.86	103.41
2	C	801	FAD	O2A-PA-O5B	-4.44	86.11	108.51
2	C	801	FAD	P-O3P-PA	-3.96	120.06	131.68
2	B	801	FAD	P-O3P-PA	-3.85	120.41	131.68
2	D	801	FAD	P-O3P-PA	-3.84	120.42	131.68
2	A	801	FAD	P-O3P-PA	-3.84	120.44	131.68
2	D	801	FAD	N3A-C4A-N9A	3.37	131.52	125.43
2	B	801	FAD	N3A-C4A-N9A	3.35	131.49	125.43
2	A	801	FAD	N3A-C4A-N9A	3.35	131.49	125.43
2	C	801	FAD	N3A-C4A-N9A	3.35	131.48	125.43
2	C	801	FAD	C4X-N5-C5X	2.72	119.74	116.69
2	B	801	FAD	C5X-C9A-N10	2.68	119.44	116.80
2	B	801	FAD	C1'-N10-C9A	2.67	121.47	118.87
2	C	801	FAD	C5X-C9A-N10	2.67	119.43	116.80
2	A	801	FAD	C5X-C9A-N10	2.66	119.42	116.80
2	C	801	FAD	C1'-N10-C9A	2.64	121.44	118.87
2	D	801	FAD	C5X-C9A-N10	2.64	119.40	116.80
2	C	801	FAD	C4X-C10-N1	-2.63	120.10	122.73
2	B	801	FAD	C4X-C10-N1	-2.63	120.10	122.73
2	C	801	FAD	C4-N3-C2	-2.63	119.99	125.39
2	B	801	FAD	C4X-N5-C5X	2.63	119.64	116.69
2	D	801	FAD	C1'-N10-C9A	2.62	121.42	118.87
2	B	801	FAD	C4-N3-C2	-2.61	120.03	125.39
2	D	801	FAD	C4-N3-C2	-2.61	120.03	125.39
2	C	801	FAD	O2A-PA-O3P	2.60	117.48	105.14
2	A	801	FAD	C1'-N10-C9A	2.60	121.40	118.87
2	A	801	FAD	C4-N3-C2	-2.60	120.06	125.39
2	D	801	FAD	C4X-N5-C5X	2.59	119.60	116.69
2	D	801	FAD	C4X-C10-N1	-2.59	120.14	122.73
2	A	801	FAD	C4X-C10-N1	-2.57	120.16	122.73
2	A	801	FAD	C4X-N5-C5X	2.57	119.58	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FAD	O4B-C1B-C2B	-2.46	103.00	106.77
2	A	801	FAD	O4B-C1B-C2B	-2.42	103.06	106.77
2	A	801	FAD	C9A-N10-C10	-2.38	119.43	121.77
2	C	801	FAD	C9A-N10-C10	-2.34	119.47	121.77
2	B	801	FAD	O4B-C1B-C2B	-2.33	103.19	106.77
2	D	801	FAD	C5A-C4A-N3A	-2.33	120.63	125.70
2	D	801	FAD	C9A-N10-C10	-2.33	119.48	121.77
2	B	801	FAD	C9A-N10-C10	-2.31	119.50	121.77
2	D	801	FAD	O4B-C1B-C2B	-2.31	103.23	106.77
2	B	801	FAD	N7A-C8A-N9A	-2.31	107.83	114.36
2	B	801	FAD	C5A-C4A-N3A	-2.31	120.68	125.70
2	D	801	FAD	N7A-C8A-N9A	-2.30	107.84	114.36
2	C	801	FAD	N7A-C8A-N9A	-2.30	107.84	114.36
2	C	801	FAD	C5A-C4A-N3A	-2.30	120.68	125.70
2	A	801	FAD	C5A-C4A-N3A	-2.30	120.68	125.70
2	A	801	FAD	N7A-C8A-N9A	-2.29	107.87	114.36
2	C	801	FAD	C4-C4X-C10	2.14	120.41	116.95
2	A	801	FAD	C4-C4X-C10	2.14	120.40	116.95
2	D	801	FAD	C4-C4X-C10	2.13	120.38	116.95
2	B	801	FAD	C4-C4X-C10	2.12	120.37	116.95
3	D	802	PG4	C2-O2-C3	2.08	119.36	112.51
2	B	801	FAD	C2A-N3A-C4A	2.03	119.80	114.01
2	D	801	FAD	C2A-N3A-C4A	2.03	119.80	114.01
2	C	801	FAD	C2A-N3A-C4A	2.03	119.80	114.01
2	A	801	FAD	C2A-N3A-C4A	2.01	119.74	114.01

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	494/516 (95%)	0.14	8 (1%) 68 69	18, 31, 53, 77	0
1	B	502/516 (97%)	0.18	11 (2%) 59 59	19, 31, 57, 80	0
1	C	488/516 (94%)	0.10	6 (1%) 75 76	18, 31, 51, 73	0
1	D	498/516 (96%)	0.17	9 (1%) 65 66	17, 30, 55, 82	0
All	All	1982/2064 (96%)	0.15	34 (1%) 67 67	17, 30, 54, 82	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	PRO	4.3
1	A	189	PHE	4.3
1	B	349	THR	3.9
1	D	421	ILE	3.8
1	A	132	GLN	3.5
1	D	230	PRO	3.5
1	B	421	ILE	3.5
1	A	232	LYS	3.4
1	B	133	HIS	3.3
1	B	231	SER	3.2
1	C	189	PHE	3.2
1	C	133	HIS	3.0
1	A	7	ALA	3.0
1	A	428	ASN	2.9
1	C	428	ASN	2.9
1	A	131	HIS	2.8
1	D	344	ASP	2.8
1	C	344	ASP	2.7
1	D	131	HIS	2.7
1	C	132	GLN	2.5
1	B	174	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	103	GLU	2.5
1	B	189	PHE	2.4
1	D	133	HIS	2.4
1	D	343	GLU	2.4
1	D	189	PHE	2.3
1	A	133	HIS	2.3
1	B	230	PRO	2.3
1	C	190	GLY	2.2
1	B	264	PRO	2.1
1	B	342	ARG	2.1
1	B	267	ASN	2.1
1	B	263	GLN	2.0
1	D	331	GLU	2.0

## 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
3	PG4	D	802	11/13	0.18	2.62	30,37,43,47	0
3	PG4	C	802	13/13	0.18	1.79	29,37,46,64	0
2	FAD	D	801	53/53	0.13	1.60	15,20,25,25	0
3	PG4	B	802	11/13	0.15	1.24	31,38,45,47	0
3	PG4	A	802	13/13	0.19	1.21	31,37,46,47	0
2	FAD	B	801	53/53	0.12	1.02	18,21,25,26	0
2	FAD	A	801	53/53	0.11	0.83	15,20,23,26	0
2	FAD	C	801	53/53	0.10	0.72	14,21,25,26	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.