



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:15 AM GMT

PDB ID : 3L1R  
Title : X-ray structure of the mutant lys300met of polyamine oxidase from zea mays  
in complex with spermidine  
Authors : Fiorillo, A.; Ilari, A.; Tavladoraki, P.  
Deposited on : 2009-12-14  
Resolution : 3.20 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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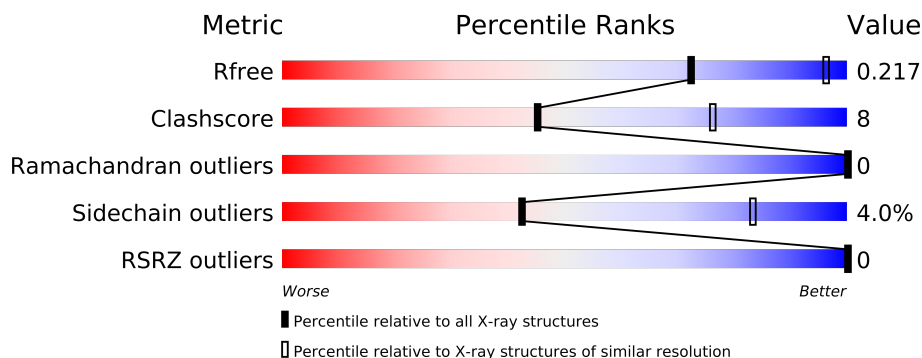
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.20 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	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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	478	
1	B	478	

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	NAG	A	600	-	X
4	SPD	B	700	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7687 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	20	0	0
			3748	2394	632	707	15			
1	B	466	Total	C	N	O	S	20	1	0
			3747	2394	633	705	15			

There are 14 discrepancies between the modelled and reference sequences:

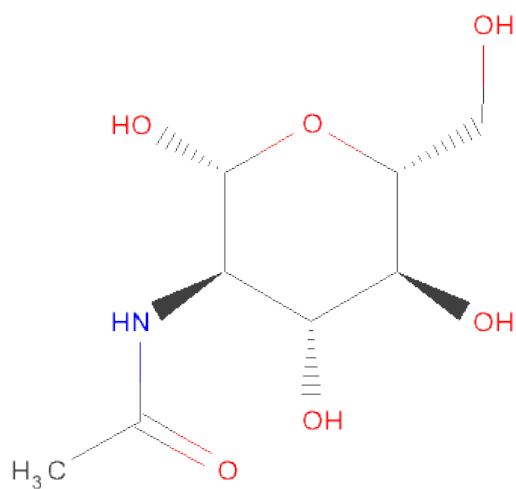
Chain	Residue	Modelled	Actual	Comment	Reference
A	300	MET	LYS	ENGINEERED	UNP O64411
A	473	HIS	-	EXPRESSION TAG	UNP O64411
A	474	HIS	-	EXPRESSION TAG	UNP O64411
A	475	HIS	-	EXPRESSION TAG	UNP O64411
A	476	HIS	-	EXPRESSION TAG	UNP O64411
A	477	HIS	-	EXPRESSION TAG	UNP O64411
A	478	HIS	-	EXPRESSION TAG	UNP O64411
B	300	MET	LYS	ENGINEERED	UNP O64411
B	473	HIS	-	EXPRESSION TAG	UNP O64411
B	474	HIS	-	EXPRESSION TAG	UNP O64411
B	475	HIS	-	EXPRESSION TAG	UNP O64411
B	476	HIS	-	EXPRESSION TAG	UNP O64411
B	477	HIS	-	EXPRESSION TAG	UNP O64411
B	478	HIS	-	EXPRESSION TAG	UNP O64411

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



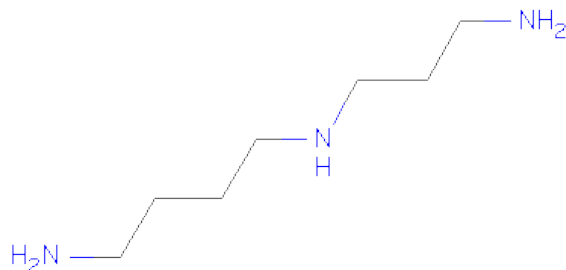
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SPERMIDINE (three-letter code: SPD) (formula:  $C_7H_{19}N_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			10	7	3		
4	B	1	Total	C	N	0	0
			10	7	3		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			28	16	2	10		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	300	MET	LYS	ENGINEERED	UNP O64411
B	473	HIS	-	EXPRESSION TAG	UNP O64411
B	474	HIS	-	EXPRESSION TAG	UNP O64411
B	475	HIS	-	EXPRESSION TAG	UNP O64411
B	476	HIS	-	EXPRESSION TAG	UNP O64411
B	477	HIS	-	EXPRESSION TAG	UNP O64411
B	478	HIS	-	EXPRESSION TAG	UNP O64411

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		

- Molecule 8 is water.

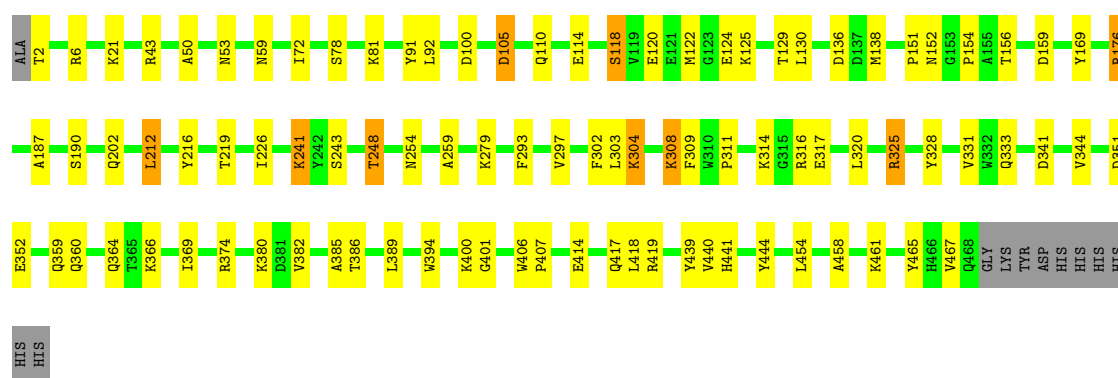
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	11	Total	O	0	0
			11	11		
8	B	7	Total	O	0	0
			7	7		

### 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.

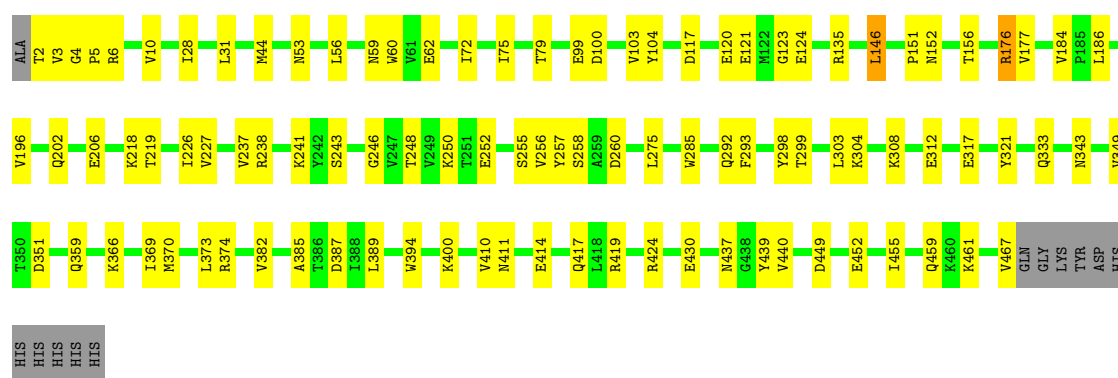
#### • Molecule 1: Polyamine oxidase

Chain A:



#### • Molecule 1: Polyamine oxidase

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.68Å 137.68Å 189.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.50 – 3.20 46.49 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.50-3.20) 100.0 (46.49-3.20)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.46 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0043	Depositor
R, $R_{free}$	0.192 , 0.216 0.197 , 0.217	Depositor DCC
$R_{free}$ test set	1749 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.5	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 11.5	EDS
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 34748 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7687	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: SO4, SPD, NAG, FAD, CL

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	0.43	0/3841	0.55	1/5207 (0.0%)
1	B	0.44	0/3843	0.55	0/5209
All	All	0.43	0/7684	0.55	1/10416 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ASP	CB-CG-OD2	5.23	123.01	118.30

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	3748	0	3645	67	0
1	B	3747	0	3650	71	0
2	A	53	0	31	2	0
2	B	53	0	31	1	0
3	A	14	0	13	0	0
4	A	10	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	10	0	19	3	0
5	B	28	0	25	0	0
6	B	5	0	0	0	0
7	B	1	0	0	0	0
8	A	11	0	0	1	0
8	B	7	0	0	0	0
All	All	7687	0	7433	126	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 8.

All (126) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:146:LEU:HD12	1:B:146:LEU:O	1.38	1.22
1:A:138:MET:HB3	1:B:292:GLN:HE21	1.13	1.09
1:B:146:LEU:HD12	1:B:146:LEU:C	1.80	0.99
1:A:138:MET:HB3	1:B:292:GLN:NE2	1.84	0.92
1:B:62:GLU:OE1	1:B:439:TYR:CE2	2.32	0.81
1:A:176:ARG:HD2	1:B:177:VAL:HG11	1.62	0.81
1:B:62:GLU:OE1	1:B:439:TYR:HE2	1.63	0.81
1:A:454:LEU:C	1:A:454:LEU:HD23	2.01	0.80
1:A:454:LEU:HD23	1:A:454:LEU:O	1.81	0.78
1:A:366:LYS:HE3	1:A:385:ALA:O	1.87	0.74
1:B:117:ASP:O	1:B:121:GLU:HG3	1.89	0.72
1:B:146:LEU:CD1	1:B:146:LEU:O	2.30	0.71
1:A:311:PRO:HB2	1:A:316:ARG:HD2	1.71	0.71
1:A:417:GLN:HG2	1:A:467:VAL:HG11	1.77	0.67
1:B:3:VAL:N	1:B:4:GLY:HA3	2.10	0.66
1:B:5:PRO:HD2	1:B:258:SER:O	1.94	0.65
1:A:308:LYS:HG2	1:A:308:LYS:O	1.98	0.64
1:B:2:THR:HG22	1:B:260:ASP:OD1	1.98	0.64
1:A:458:ALA:O	1:A:461:LYS:HE3	1.98	0.63
1:A:454:LEU:C	1:A:454:LEU:CD2	2.67	0.62
1:A:212:LEU:HD21	1:A:444:TYR:HE1	1.65	0.61
1:A:53:ASN:H	1:A:202:GLN:NE2	1.98	0.61
1:A:400:LYS:HB3	1:B:151:PRO:HG3	1.82	0.60
1:B:146:LEU:CD1	1:B:146:LEU:C	2.58	0.60
1:A:414:GLU:HA	1:A:417:GLN:HG3	1.82	0.60
1:B:3:VAL:H	1:B:4:GLY:HA3	1.67	0.59
1:A:138:MET:CB	1:B:292:GLN:HE21	2.02	0.58
1:B:410:VAL:HG13	1:B:414:GLU:HG3	1.85	0.58
1:B:219:THR:HG22	1:B:226:ILE:HA	1.85	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:6[A]:ARG:NH1	1:B:260:ASP:CG	2.57	0.57
1:B:299:THR:HB	1:B:349:VAL:HG23	1.87	0.57
1:B:124:GLU:HG3	1:B:184:VAL:HG12	1.86	0.56
1:A:394:TRP:HE1	1:B:152:ASN:ND2	2.03	0.56
1:B:60:TRP:CZ3	4:B:700:SPD:H41	2.40	0.56
1:A:53:ASN:H	1:A:202:GLN:HE22	1.52	0.56
1:A:302:PHE:HB2	1:A:389:LEU:HB3	1.88	0.55
1:A:130:LEU:HD22	1:A:136:ASP:O	2.06	0.55
1:A:78:SER:O	1:A:81:LYS:HE2	2.07	0.55
1:A:212:LEU:HD21	1:A:444:TYR:CE1	2.42	0.54
1:A:359:GLN:HE22	1:B:156:THR:HG22	1.72	0.54
1:B:6[B]:ARG:HG2	1:B:28:ILE:HG23	1.89	0.54
1:B:241:LYS:HB2	1:B:248:THR:HB	1.89	0.54
1:B:62:GLU:HG2	1:B:196:VAL:CG1	2.38	0.54
1:A:303:LEU:HD11	1:A:369:ILE:HG21	1.90	0.53
1:B:370:MET:HE1	1:B:373:LEU:HD12	1.90	0.53
1:B:99:GLU:HA	1:B:321:TYR:CE1	2.44	0.53
1:A:325:ARG:HD2	1:A:328:TYR:HB2	1.91	0.53
1:B:298:TYR:OH	4:B:700:SPD:H51	2.09	0.53
1:B:255:SER:HB3	1:B:257:TYR:CE1	2.45	0.52
1:A:50:ALA:CB	1:A:304:LYS:HD2	2.40	0.51
1:A:394:TRP:HE1	1:B:152:ASN:HD22	1.58	0.51
1:B:218:LYS:HG3	1:B:227:VAL:HG23	1.93	0.51
1:B:250:LYS:HG2	1:B:256:VAL:HG22	1.92	0.51
1:B:6[A]:ARG:HH12	1:B:260:ASP:CG	2.15	0.50
1:A:176:ARG:NH2	1:B:351:ASP:OD1	2.40	0.50
2:A:500:FAD:O2A	8:A:487:HOH:O	2.19	0.50
1:A:110:GLN:HE21	1:A:114:GLU:HG3	1.75	0.49
1:A:151:PRO:HG3	1:B:400:LYS:HB3	1.95	0.49
1:A:419:ARG:NH2	1:A:465:TYR:OH	2.45	0.49
1:A:118:SER:O	1:A:122:MET:HG3	2.13	0.49
1:A:187:ALA:HA	1:A:190:SER:HB2	1.95	0.48
1:B:75:ILE:HA	1:B:79:THR:HB	1.96	0.48
1:A:72:ILE:HD13	1:A:441:HIS:HA	1.95	0.48
1:A:351:ASP:CG	1:A:352:GLU:H	2.15	0.48
1:B:62:GLU:HG2	1:B:196:VAL:HG11	1.96	0.47
1:A:50:ALA:HB1	1:A:304:LYS:HD2	1.96	0.47
1:B:246:GLY:HA2	1:B:424:ARG:CD	2.44	0.47
1:A:72:ILE:HG12	1:A:440:VAL:HG12	1.96	0.47
1:B:308:LYS:HE2	1:B:343:ASN:OD1	2.14	0.47
1:B:2:THR:HA	1:B:260:ASP:OD1	2.13	0.47
1:A:359:GLN:NE2	1:B:156:THR:HG22	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:92:LEU:HD22	1:A:320:LEU:HG	1.97	0.47
1:A:351:ASP:CG	1:B:176:ARG:HH22	2.19	0.46
1:B:6[B]:ARG:HG2	1:B:28:ILE:CG2	2.45	0.46
1:B:303:LEU:HD11	1:B:369:ILE:HG21	1.98	0.46
1:B:455:ILE:O	1:B:459:GLN:HB3	2.16	0.46
1:A:91:TYR:OH	1:A:314:LYS:HE2	2.16	0.46
1:A:309:PHE:CG	1:A:382:VAL:HG12	2.50	0.46
1:B:62:GLU:OE1	1:B:439:TYR:CD2	2.70	0.45
1:B:10:VAL:HG22	1:B:237:VAL:HG21	1.97	0.45
1:A:125:LYS:O	1:A:129:THR:HG23	2.17	0.45
1:B:56:LEU:HD21	1:B:389:LEU:HD21	1.98	0.45
1:B:366:LYS:HD2	1:B:385:ALA:HB3	1.98	0.45
1:A:241:LYS:HA	1:A:279:LYS:O	2.17	0.45
1:A:120:GLU:O	1:A:124:GLU:HG3	2.16	0.45
1:A:136:ASP:N	1:A:136:ASP:OD1	2.50	0.45
1:A:374:ARG:HE	1:A:382:VAL:HG23	1.81	0.44
1:A:151:PRO:HG2	1:A:152:ASN:HD22	1.83	0.44
1:B:186:LEU:HD21	1:B:439:TYR:OH	2.18	0.44
1:A:241:LYS:HG3	1:A:279:LYS:HB3	1.98	0.44
1:B:238:ARG:HG3	1:B:252:GLU:HG3	1.98	0.44
1:B:103:VAL:HG12	1:B:104:TYR:O	2.18	0.44
1:A:169:TYR:CE1	1:A:331:VAL:HG11	2.52	0.44
1:A:303:LEU:O	1:A:344:VAL:HA	2.18	0.43
1:B:298:TYR:CZ	4:B:700:SPD:H51	2.52	0.43
1:B:452:GLU:HA	1:B:455:ILE:HD12	1.99	0.43
1:B:285:TRP:HE3	1:B:417:GLN:HE21	1.66	0.43
1:A:439:TYR:HB3	1:A:441:HIS:CE1	2.52	0.43
1:A:297:VAL:HG22	1:A:401:GLY:HA2	1.99	0.43
1:A:351:ASP:CG	1:A:352:GLU:N	2.72	0.43
1:A:219:THR:HG22	1:A:226:ILE:HA	2.00	0.43
1:B:238:ARG:CG	1:B:252:GLU:HG3	2.49	0.42
1:A:72:ILE:CD1	1:A:441:HIS:HA	2.49	0.42
1:B:72:ILE:HG13	1:B:440:VAL:HG12	2.01	0.42
1:A:21:LYS:HB2	1:A:216:TYR:CE2	2.55	0.42
1:A:105:ASP:OD1	1:A:105:ASP:N	2.52	0.42
1:B:6[A]:ARG:NH1	1:B:260:ASP:OD2	2.53	0.42
1:A:43:ARG:HB3	2:A:500:FAD:HM81	2.02	0.42
1:B:308:LYS:HD2	1:B:312:GLU:OE1	2.20	0.41
1:A:317:GLU:O	1:A:333:GLN:HA	2.20	0.41
1:B:317:GLU:O	1:B:333:GLN:HA	2.20	0.41
1:A:406:TRP:HA	1:A:407:PRO:HD3	1.89	0.41
1:A:154:PRO:HB3	1:A:159:ASP:HB3	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:6:ARG:O	1:A:259:ALA:HB1	2.20	0.41
1:B:394:TRP:O	1:B:400:LYS:HA	2.21	0.41
1:B:430:GLU:O	1:B:437:ASN:HA	2.21	0.41
1:A:297:VAL:HG21	1:A:394:TRP:HB2	2.03	0.41
1:A:241:LYS:HB3	1:A:248:THR:HB	2.02	0.41
1:B:304:LYS:HB3	1:B:387:ASP:HB2	2.03	0.41
1:A:304:LYS:HG3	1:A:386:THR:OG1	2.21	0.40
1:B:275:LEU:CD2	2:B:500:FAD:H61A	2.34	0.40
1:B:44:MET:O	1:B:206:GLU:HB3	2.21	0.40
1:B:374:ARG:HG2	1:B:382:VAL:HB	2.03	0.40
1:B:53:ASN:H	1:B:202:GLN:HE22	1.68	0.40
1:A:156:THR:HG22	1:B:359:GLN:HE22	1.85	0.40
1:B:120:GLU:O	1:B:123:GLY:N	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	465/478 (97%)	441 (95%)	24 (5%)	0	100	100
1	B	465/478 (97%)	441 (95%)	24 (5%)	0	100	100
All	All	930/956 (97%)	882 (95%)	48 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	401/410 (98%)	382 (95%)	19 (5%)	36	79
1	B	401/410 (98%)	388 (97%)	13 (3%)	51	87
All	All	802/820 (98%)	770 (96%)	32 (4%)	42	83

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	59	ASN
1	A	100	ASP
1	A	105	ASP
1	A	118	SER
1	A	176	ARG
1	A	212	LEU
1	A	241	LYS
1	A	243	SER
1	A	248	THR
1	A	254	ASN
1	A	293	PHE
1	A	304	LYS
1	A	308	LYS
1	A	325	ARG
1	A	360	GLN
1	A	364	GLN
1	A	380	LYS
1	A	418	LEU
1	B	31	LEU
1	B	59	ASN
1	B	100	ASP
1	B	135	ARG
1	B	146	LEU
1	B	176	ARG
1	B	243	SER
1	B	293	PHE
1	B	411	ASN
1	B	419	ARG
1	B	449	ASP
1	B	461	LYS
1	B	467	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	110	GLN
1	A	149	HIS
1	A	152	ASN
1	A	202	GLN
1	A	359	GLN
1	A	360	GLN
1	A	456	ASN
1	A	466	HIS
1	B	152	ASN
1	B	202	GLN
1	B	215	GLN
1	B	277	GLN
1	B	292	GLN
1	B	359	GLN
1	B	360	GLN
1	B	435	HIS
1	B	437	ASN

### 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 ⓘ

2 carbohydrates 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	$\# Z  > 2$
5	NAG	B	600	1,5	12,14,15	0.55	0	15,19,21	1.48	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	B	601	5	12,14,15	0.79	1 (8%)	15,19,21	1.43	3 (20%)

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
5	NAG	B	600	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	601	5	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	NAG	O5-C5	-2.14	1.41	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	600	NAG	O5-C5-C6	4.59	111.80	106.98
5	B	601	NAG	O5-C5-C4	-2.76	107.15	110.65
5	B	601	NAG	C4-C3-C2	2.70	117.93	111.32
5	B	601	NAG	C3-C2-N2	-2.67	107.69	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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	500	-	58,58,58	1.00	4 (6%)	85,89,89	1.87	17 (20%)
3	NAG	A	600	1	12,14,15	0.62	0	15,19,21	1.86	3 (20%)
4	SPD	A	700	-	9,9,9	0.29	0	8,8,8	0.85	0
6	SO4	B	479	-	4,4,4	0.18	0	6,6,6	0.25	0
2	FAD	B	500	-	58,58,58	1.03	4 (6%)	85,89,89	1.94	16 (18%)
4	SPD	B	700	-	9,9,9	0.31	0	8,8,8	0.74	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	500	-	-	0/34/50/50	0/1/6/6
3	NAG	A	600	1	-	0/6/23/26	0/1/1/1
4	SPD	A	700	-	-	0/7/7/7	0/0/0/0
6	SO4	B	479	-	-	0/0/0/0	0/0/0/0
2	FAD	B	500	-	-	0/34/50/50	0/1/6/6
4	SPD	B	700	-	-	0/7/7/7	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	FAD	C2A-N3A	3.33	1.38	1.32
2	A	500	FAD	C2A-N3A	3.12	1.38	1.32
2	B	500	FAD	C2A-N1A	2.62	1.39	1.33
2	A	500	FAD	C2A-N1A	2.46	1.38	1.33
2	B	500	FAD	C5X-N5	2.34	1.38	1.35
2	A	500	FAD	C1'-N10	2.27	1.50	1.48
2	B	500	FAD	C10-N1	2.19	1.39	1.35
2	A	500	FAD	C5X-N5	2.15	1.38	1.35

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	FAD	N3A-C2A-N1A	-10.72	119.74	128.71
2	B	500	FAD	N3A-C2A-N1A	-10.70	119.76	128.71
2	B	500	FAD	C2-N1-C10	5.91	120.93	114.98
2	A	500	FAD	C2-N1-C10	5.51	120.53	114.98
3	A	600	NAG	O5-C5-C6	5.37	112.61	106.98
2	B	500	FAD	C4X-N5-C5X	4.66	121.92	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	FAD	C4X-C10-N1	-3.79	118.95	122.73
2	B	500	FAD	N3A-C4A-N9A	3.65	132.01	125.43
2	B	500	FAD	C4X-C10-N10	-3.44	118.79	120.51
2	B	500	FAD	C4A-C5A-N7A	-3.35	106.65	109.52
2	A	500	FAD	N3A-C4A-N9A	3.32	131.43	125.43
2	B	500	FAD	C4X-C10-N1	-3.27	119.46	122.73
2	B	500	FAD	P-O3P-PA	-3.18	122.36	131.68
2	B	500	FAD	C5'-C4'-C3'	-3.15	106.11	112.06
2	A	500	FAD	C5'-C4'-C3'	-3.11	106.19	112.06
2	B	500	FAD	O4B-C1B-N9A	2.95	111.19	108.44
2	A	500	FAD	O4B-C1B-N9A	2.94	111.17	108.44
2	A	500	FAD	C4-N3-C2	-2.89	119.47	125.39
2	A	500	FAD	C5X-C9A-N10	2.87	119.63	116.80
2	A	500	FAD	P-O3P-PA	-2.83	123.40	131.68
3	A	600	NAG	O5-C5-C4	-2.76	107.15	110.65
2	A	500	FAD	C1B-N9A-C4A	-2.73	121.92	126.64
2	B	500	FAD	C9A-C5X-N5	-2.70	118.23	122.37
2	A	500	FAD	C4A-C5A-N7A	-2.65	107.25	109.52
2	A	500	FAD	C4X-N5-C5X	2.65	119.67	116.69
2	B	500	FAD	C5A-C4A-N3A	-2.46	120.35	125.70
2	B	500	FAD	C5X-C9A-N10	2.36	119.12	116.80
2	A	500	FAD	N7A-C8A-N9A	-2.34	107.73	114.36
2	B	500	FAD	C4-N3-C2	-2.33	120.61	125.39
2	A	500	FAD	C1'-N10-C9A	2.21	121.03	118.87
3	A	600	NAG	C3-C2-N2	-2.11	108.55	111.76
2	A	500	FAD	C9A-N10-C10	-2.10	119.71	121.77
2	A	500	FAD	C5A-C4A-N3A	-2.09	121.15	125.70
2	A	500	FAD	C4X-C10-N10	-2.07	119.48	120.51
2	B	500	FAD	C2A-N3A-C4A	2.05	119.85	114.01
2	B	500	FAD	C10-C4X-N5	-2.03	117.98	120.45

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	467/478 (97%)	-0.25	0 100 100	20, 29, 39, 52	21 (4%)
1	B	466/478 (97%)	-0.25	0 100 100	19, 29, 39, 51	13 (2%)
All	All	933/956 (97%)	-0.25	0 100 100	19, 29, 39, 52	34 (3%)

There are no RSRZ outliers to report.

### 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 ⓘ

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
5	NAG	B	600	14/15	0.36	0.86	51,53,55,58	0
5	NAG	B	601	14/15	0.52	-	60,62,63,63	0

### 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( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	600	14/15	0.41	6.35	45,48,49,50	0
4	SPD	B	700	10/10	0.25	4.00	34,36,40,40	0
4	SPD	A	700	10/10	0.18	1.06	33,39,42,43	0
2	FAD	B	500	53/53	0.15	-0.06	22,25,27,27	0
2	FAD	A	500	53/53	0.14	-0.32	18,22,25,27	0
6	SO4	B	479	5/5	0.17	-0.76	54,54,54,55	0
7	CL	B	480	1/1	0.11	-1.90	31,31,31,31	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.