



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:30 am GMT

PDB ID : 1H81  
Title : STRUCTURE OF POLYAMINE OXIDASE IN THE REDUCED STATE  
Authors : Binda, C.; Coda, A.; Angelini, R.; Federico, R.; Ascenzi, P.; Mattevi, A.  
Deposited on : 2001-01-24  
Resolution : 2.10 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

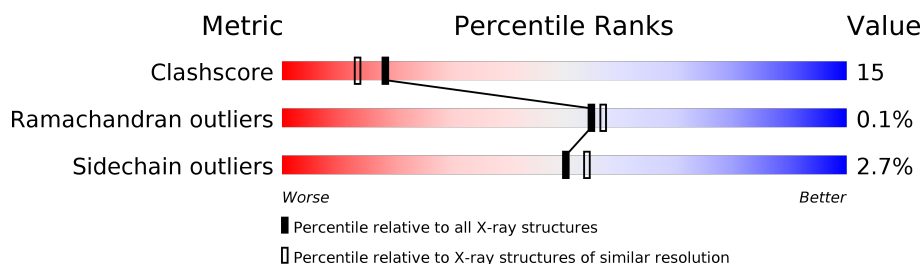
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	472	<div> <div>66%</div> <div>29%</div> <div>..</div> </div>
1	B	472	<div> <div>70%</div> <div>26%</div> <div>..</div> </div>
1	C	472	<div> <div>71%</div> <div>26%</div> <div>..</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
5	MAN	C	604	X	-	-	-

## 2 Entry composition [i](#)

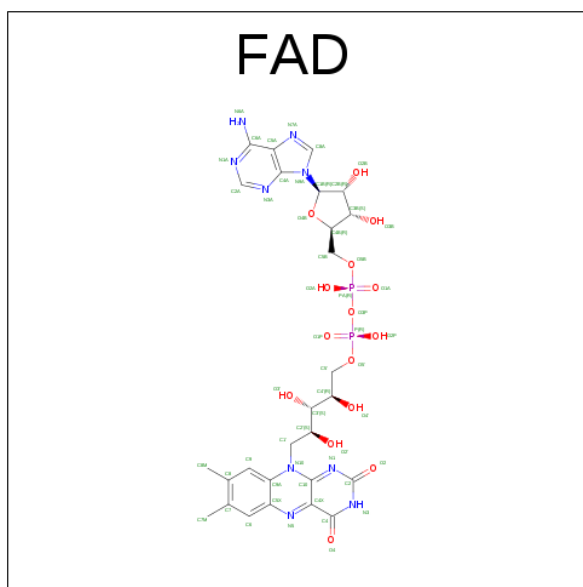
There are 6 unique types of molecules in this entry. The entry contains 12113 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 POLYAMINE OXIDASE.

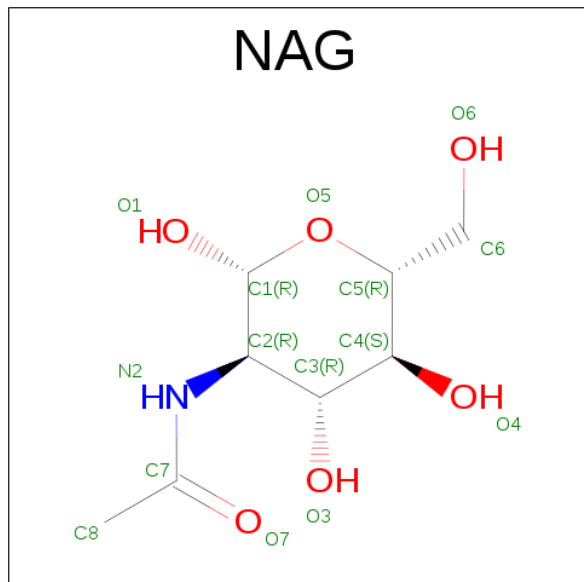
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	55	0	0
			3684	2353	621	696	14			
1	B	462	Total	C	N	O	S	61	0	0
			3715	2374	627	700	14			
1	C	462	Total	C	N	O	S	50	0	0
			3715	2374	627	700	14			

- 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		

- 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		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	2	Total	C	N	O	0	0
			24	14	1	9		

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	2	Total	C	O	0	0
			22	12	10		

- Molecule 6 is water.

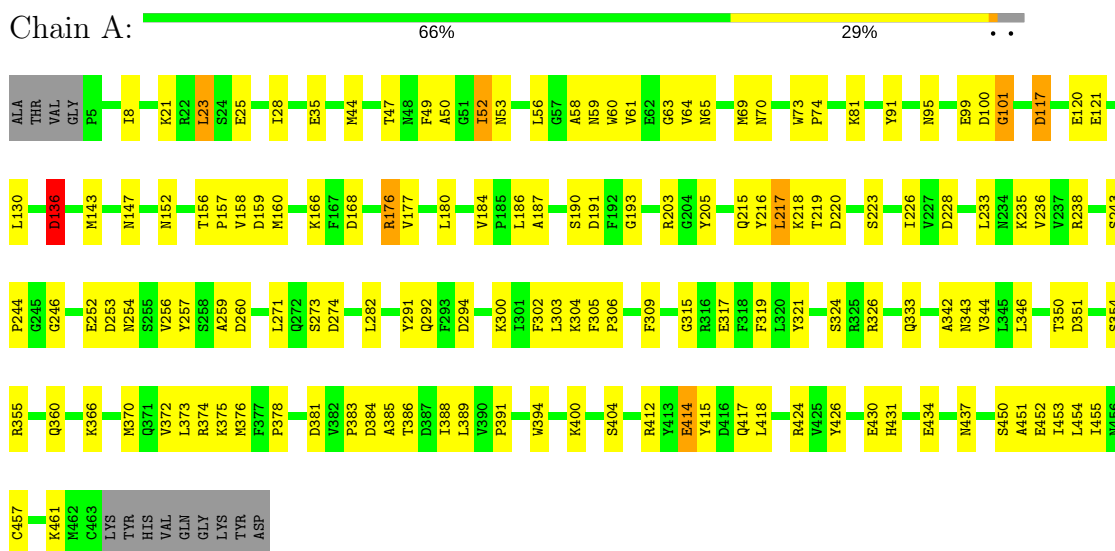
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	224	Total 224	O 224	0	0
6	B	245	Total 245	O 245	0	0
6	C	255	Total 255	O 255	0	0

### 3 Residue-property plots

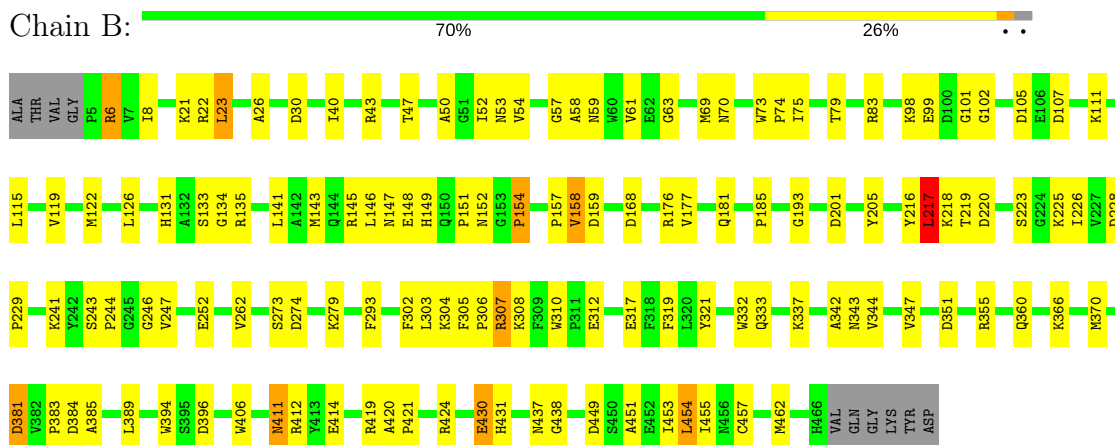
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

#### • Molecule 1: POLYAMINE OXIDASE



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ALA	D117	K241	K376
THR	S118	T242	M376
VAL	V119	S243	F377
GLY	E120	P244	P378
P5	E121	G245	P383
R6	M122	G246	D384
V7			A385
I8	S127	K250	
		T251	
K21	H131	E252	L389
R22	A132	D253	
L23	S133	N254	R397
S24		S255	
E25	R145	V256	T402
A26	L146	Y257	
G27	N147	S258	N405
I28		A259	
T29	P154		R412
D30		S273	
	V158		L418
E35	D159	K279	R419
N48	E173	L282	R424
F49			
A50	R176	V285	E430
G51		K286	H431
	A187	V287	E434
G57		R288	
A58	S190	A289	N437
N59	D191	I290	G438
V60	F192	V291	Y439
V61	G193	Q292	V440
E62		F293	H441
G63	F198	D294	
V64			I455
N65	Y205	F302	N456
G66		L303	C457
	A213	K304	
R69			K461
N70	Y216	R307	
	L217		H466
W73	K218	E317	VAL
P74	T219		GLN
	D220		GLY
	D221	Q333	LYS
Y91	K222		TYR
	S223	Y339	ASP
V96		P340	
	G224	D341	
G101	K225	A342	
G102	I226	N343	
V103	V227	V344	
Y104	D228		
D105	P229	R355	
E106	R230		
D107		K366	
	L233		
R112		M370	
	R238		
L115	E239		
A116	I240	R374	

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.77Å 181.77Å 277.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	99.1 (20.00-2.10)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT 5D	Depositor
R, $R_{free}$	0.191 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12113	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FCA, NAG, FAD, MAN

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	0.54	0/3775	1.30	16/5116 (0.3%)
1	B	0.53	0/3808	1.26	15/5160 (0.3%)
1	C	0.55	0/3808	1.29	21/5160 (0.4%)
All	All	0.54	0/11391	1.28	52/15436 (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	C	1	0
5	C	1	0
All	All	2	0

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	355	ARG	NE-CZ-NH2	-12.67	113.97	120.30
1	A	117	ASP	CB-CG-OD1	-10.79	108.59	118.30
1	C	230	ARG	NE-CZ-NH1	-10.74	114.93	120.30
1	C	145	ARG	NE-CZ-NH2	-10.13	115.24	120.30
1	B	135	ARG	NE-CZ-NH1	-9.11	115.74	120.30
1	B	355	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	C	145	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	C	112	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	C	307	ARG	NE-CZ-NH1	-7.40	116.60	120.30
1	C	355	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	101	GLY	N-CA-C	7.15	130.99	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	22	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	C	176	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	355	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	61	VAL	N-CA-C	-6.79	92.66	111.00
1	B	252	GLU	N-CA-CB	-6.60	98.72	110.60
1	C	115	LEU	CB-CG-CD1	-6.59	99.79	111.00
1	C	6	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	351	ASP	N-CA-CB	-6.20	99.44	110.60
1	B	61	VAL	N-CA-C	-6.18	94.32	111.00
1	A	260	ASP	CB-CG-OD2	6.11	123.80	118.30
1	C	397	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	136	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	C	105	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	326	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	A	351	ASP	N-CA-CB	-6.03	99.74	110.60
1	C	374	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	C	61	VAL	N-CA-C	-5.85	95.21	111.00
1	A	60	TRP	CB-CA-C	-5.82	98.77	110.40
1	A	374	ARG	NE-CZ-NH1	-5.79	117.41	120.30
1	B	307	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	43	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	C	273	SER	C-N-CA	-5.62	107.64	121.70
1	A	56	LEU	CB-CG-CD2	-5.62	101.45	111.00
1	A	176	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	414	GLU	CA-CB-CG	-5.54	101.22	113.40
1	C	340	PRO	C-N-CA	-5.52	107.90	121.70
1	C	282	LEU	CB-CG-CD1	5.49	120.34	111.00
1	B	396	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	B	126	LEU	CB-CG-CD2	-5.40	101.81	111.00
1	B	201	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	B	217	LEU	CB-CG-CD2	-5.38	101.86	111.00
1	C	307	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	C	397	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	6	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	C	288	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	A	381	ASP	N-CA-C	-5.20	96.97	111.00
1	C	341	ASP	CB-CA-C	5.15	120.69	110.40
1	B	101	GLY	N-CA-C	5.14	125.94	113.10
1	B	381	ASP	N-CA-C	-5.13	97.14	111.00
1	A	44	MET	N-CA-C	-5.04	97.38	111.00
1	C	418	LEU	CB-CA-C	-5.01	100.68	110.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	386	THR	CB
5	C	604	MAN	C1

There are no planarity outliers.

## 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	3684	0	3584	113	0
1	B	3715	0	3614	110	0
1	C	3715	0	3614	99	0
2	A	53	0	31	2	0
2	B	53	0	31	2	0
2	C	53	0	31	5	0
3	A	28	0	26	3	0
3	B	28	0	26	4	0
3	C	14	0	12	4	0
4	C	24	0	22	6	0
5	C	22	0	18	0	0
6	A	224	0	0	4	0
6	B	245	0	0	10	0
6	C	255	0	0	5	0
All	All	12113	0	11009	326	0

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 15.

All (326) 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:B:69:MET:CE	1:B:73:TRP:HB3	1.81	1.11
1:A:373:LEU:HD23	1:A:376:MET:HE3	1.34	1.08
1:B:69:MET:HE2	1:B:74:PRO:HD3	1.35	1.03
1:A:69:MET:CE	1:A:73:TRP:HB3	1.90	1.02
1:B:69:MET:HE3	1:B:73:TRP:HB3	1.44	0.99
4:C:601:NAG:C4	3:C:602:NAG:C1	2.41	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:HIS:CD2	1:C:133:SER:H	1.83	0.97
1:B:411:ASN:ND2	1:B:414:GLU:H	1.66	0.93
1:B:69:MET:CE	1:B:74:PRO:HD3	2.01	0.90
1:A:394:TRP:HE1	1:B:152:ASN:ND2	1.70	0.89
1:A:372:VAL:HG12	1:A:376:MET:CE	2.03	0.89
1:A:69:MET:HE2	1:A:74:PRO:HD3	1.54	0.89
1:A:69:MET:HE3	1:A:73:TRP:HB3	1.54	0.87
3:B:601:NAG:C4	3:B:602:NAG:C1	2.54	0.86
1:A:372:VAL:HG12	1:A:376:MET:HE2	1.55	0.85
1:B:219:THR:HG22	1:B:226:ILE:HA	1.59	0.84
1:B:119:VAL:HA	1:B:122:MET:HE3	1.57	0.84
1:C:112:ARG:HD3	1:C:159:ASP:OD1	1.77	0.84
1:C:216:TYR:CE1	1:C:217:LEU:HD13	2.13	0.84
1:B:308:LYS:HE3	1:B:310:TRP:O	1.76	0.83
1:B:220:ASP:HB3	1:B:223:SER:OG	1.81	0.80
3:A:601:NAG:C4	3:A:602:NAG:C1	2.60	0.80
1:C:117:ASP:O	1:C:121:GLU:HG3	1.82	0.80
1:C:69:MET:HE3	1:C:70:ASN:H	1.47	0.78
1:C:216:TYR:CD1	1:C:217:LEU:HD13	2.18	0.78
1:A:366:LYS:HD2	1:A:385:ALA:HB3	1.66	0.76
4:C:601:NAG:H3	4:C:603:FCA:O2	1.84	0.76
1:B:131:HIS:CD2	1:B:133:SER:H	2.03	0.75
1:C:220:ASP:HB3	1:C:223:SER:OG	1.86	0.75
1:A:394:TRP:HE1	1:B:152:ASN:HD22	1.35	0.75
1:A:431:HIS:H	1:A:431:HIS:CD2	2.03	0.75
1:A:50:ALA:HB1	1:A:304:LYS:HD2	1.69	0.75
1:C:131:HIS:HD2	1:C:133:SER:H	1.35	0.74
1:A:69:MET:CE	1:A:74:PRO:HD3	2.16	0.74
4:C:601:NAG:O4	3:C:602:NAG:C2	2.35	0.74
1:A:117:ASP:O	1:A:121:GLU:HG3	1.88	0.73
1:B:411:ASN:HD22	1:B:414:GLU:H	1.37	0.72
1:C:69:MET:HE3	1:C:69:MET:HA	1.71	0.72
1:C:292:GLN:OE1	6:C:2137:HOH:O	2.07	0.72
1:A:23:LEU:HD13	1:A:451:ALA:HB1	1.71	0.71
1:B:131:HIS:HD2	1:B:133:SER:H	1.38	0.71
1:B:419:ARG:HG2	6:B:2227:HOH:O	1.90	0.71
1:B:419:ARG:HD3	6:B:2218:HOH:O	1.90	0.71
1:C:69:MET:HE3	1:C:70:ASN:N	2.06	0.70
1:A:220:ASP:HB3	1:A:223:SER:HB3	1.72	0.70
1:B:216:TYR:CD1	1:B:217:LEU:HD13	2.27	0.70
1:A:218:LYS:H	1:A:228:ASP:HB2	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLY:HA2	1:A:193:GLY:O	1.93	0.69
1:B:107:ASP:O	1:B:111:LYS:HG3	1.93	0.69
1:C:131:HIS:HD2	1:C:133:SER:OG	1.76	0.69
1:C:6:ARG:HH11	1:C:6:ARG:HG3	1.57	0.69
1:A:117:ASP:OD1	6:A:2050:HOH:O	2.11	0.68
1:B:185:PRO:HA	6:B:2054:HOH:O	1.94	0.68
1:C:69:MET:CE	1:C:70:ASN:N	2.58	0.67
1:A:273:SER:O	1:A:274:ASP:HB2	1.94	0.67
1:C:131:HIS:HD2	1:C:133:SER:CB	2.07	0.66
1:B:449:ASP:O	1:B:453:ILE:HG13	1.97	0.65
1:A:372:VAL:HG12	1:A:376:MET:HE1	1.79	0.65
1:A:158:VAL:HG13	1:A:159:ASP:N	2.13	0.64
4:C:601:NAG:H4	3:C:602:NAG:C1	2.28	0.64
1:B:412:ARG:HG3	6:B:2215:HOH:O	1.96	0.64
1:C:69:MET:CE	1:C:70:ASN:H	2.11	0.64
1:A:216:TYR:CD1	1:A:217:LEU:HD13	2.31	0.64
1:A:412:ARG:NH1	1:A:434:GLU:OE2	2.30	0.64
1:B:63:GLY:HA2	1:B:193:GLY:O	1.98	0.62
1:A:58:ALA:HA	2:A:579:FAD:C4X	2.30	0.62
4:C:601:NAG:O6	3:C:602:NAG:C1	2.48	0.61
1:A:220:ASP:CB	1:A:223:SER:HB3	2.29	0.61
1:A:220:ASP:CG	1:A:223:SER:HB3	2.21	0.61
4:C:601:NAG:C3	4:C:603:FCA:O2	2.48	0.61
1:A:130:LEU:HD22	1:A:136:ASP:HB2	1.82	0.60
1:C:131:HIS:CD2	1:C:133:SER:OG	2.53	0.60
1:C:220:ASP:OD2	1:C:222:LYS:N	2.34	0.60
1:C:419:ARG:NH2	1:C:434:GLU:HA	2.17	0.60
1:C:131:HIS:CD2	1:C:133:SER:CB	2.85	0.60
1:C:431:HIS:CD2	1:C:431:HIS:H	2.18	0.60
1:A:49:PHE:N	1:A:52:ILE:O	2.30	0.60
1:A:177:VAL:HG11	1:B:176:ARG:HD2	1.83	0.59
1:C:412:ARG:NH1	1:C:434:GLU:OE2	2.33	0.59
3:B:601:NAG:O4	3:B:602:NAG:C2	2.47	0.59
1:A:152:ASN:ND2	1:B:394:TRP:HE1	2.01	0.59
1:C:69:MET:HE2	1:C:70:ASN:O	2.03	0.58
1:A:218:LYS:N	1:A:228:ASP:HB2	2.18	0.58
1:C:219:THR:HG22	1:C:226:ILE:HA	1.85	0.58
1:B:69:MET:HE2	1:B:70:ASN:O	2.04	0.58
1:B:431:HIS:H	1:B:431:HIS:CD2	2.20	0.58
1:B:26:ALA:HB2	1:B:455:ILE:HD13	1.85	0.58
1:B:273:SER:O	1:B:274:ASP:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:MET:HE3	1:C:69:MET:CA	2.35	0.57
1:B:304:LYS:HG3	1:B:305:PHE:N	2.20	0.57
1:C:6:ARG:HA	1:C:30:ASP:O	2.04	0.57
1:B:243:SER:HB2	1:B:244:PRO:CD	2.35	0.57
1:C:131:HIS:HD2	1:C:133:SER:N	2.03	0.57
1:A:243:SER:HB2	1:A:244:PRO:CD	2.34	0.56
1:A:342:ALA:O	1:A:343:ASN:HB2	2.04	0.56
1:A:50:ALA:CB	1:A:304:LYS:HD2	2.36	0.56
1:C:101:GLY:HA3	1:C:378:PRO:HG3	1.87	0.56
1:B:6:ARG:HA	1:B:30:ASP:O	2.06	0.56
1:C:218:LYS:H	1:C:228:ASP:HB2	1.71	0.56
1:B:216:TYR:CE1	1:B:217:LEU:HD13	2.41	0.56
1:A:219:THR:HG22	1:A:226:ILE:HA	1.89	0.55
1:B:23:LEU:HD13	1:B:451:ALA:HB1	1.88	0.55
1:B:58:ALA:HA	2:B:579:FAD:C4X	2.36	0.55
1:B:119:VAL:CA	1:B:122:MET:HE3	2.32	0.55
1:B:457:CYS:HA	1:B:462:MET:O	2.07	0.55
1:A:47:THR:O	1:A:53:ASN:HA	2.07	0.54
1:A:64:VAL:HG12	1:A:65:ASN:N	2.21	0.54
1:C:290:ILE:HA	1:C:418:LEU:HD21	1.89	0.54
1:B:454:LEU:C	1:B:454:LEU:HD12	2.28	0.54
1:C:219:THR:HA	1:C:225:LYS:O	2.07	0.54
1:C:253:ASP:O	1:C:254:ASN:HB2	2.08	0.54
1:B:119:VAL:HA	1:B:122:MET:CE	2.33	0.54
1:C:58:ALA:HA	2:C:579:FAD:C4X	2.38	0.54
1:B:223:SER:HB2	1:B:225:LYS:HG3	1.89	0.53
1:B:306:PRO:HG3	1:B:383:PRO:HB2	1.90	0.53
1:C:158:VAL:HG12	6:C:2073:HOH:O	2.06	0.53
1:A:216:TYR:CE1	1:A:217:LEU:HD13	2.43	0.53
1:B:69:MET:HE1	1:B:73:TRP:HB3	1.84	0.53
1:C:105:ASP:OD1	1:C:107:ASP:HB2	2.09	0.53
1:C:131:HIS:CD2	1:C:133:SER:N	2.65	0.52
1:A:156:THR:O	1:A:160:MET:HG3	2.09	0.52
1:B:131:HIS:HD2	1:B:133:SER:OG	1.93	0.52
1:C:35:GLU:HB3	1:C:233:LEU:HD23	1.90	0.52
1:A:143:MET:SD	1:A:147:ASN:ND2	2.83	0.52
1:B:98:LYS:HG3	1:B:102:GLY:O	2.10	0.52
1:C:21:LYS:HB2	1:C:216:TYR:CE2	2.45	0.52
1:C:112:ARG:NH2	1:C:115:LEU:HD11	2.24	0.52
1:C:246:GLY:HA2	1:C:424:ARG:HD3	1.92	0.51
1:C:376:MET:C	1:C:378:PRO:HD3	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASP:O	1:A:254:ASN:HB2	2.11	0.51
1:B:99:GLU:HA	1:B:321:TYR:CE1	2.46	0.51
1:C:57:GLY:HA2	2:C:579:FAD:C7M	2.41	0.51
1:A:317:GLU:O	1:A:333:GLN:HA	2.10	0.51
3:A:601:NAG:H4	3:A:602:NAG:C1	2.39	0.51
1:A:69:MET:HE2	1:A:70:ASN:O	2.10	0.51
1:B:219:THR:HG22	1:B:226:ILE:CA	2.37	0.51
1:B:342:ALA:O	1:B:343:ASN:HB2	2.11	0.51
1:C:119:VAL:HG13	1:C:147:ASN:HB2	1.93	0.51
1:C:73:TRP:HB3	1:C:74:PRO:HD3	1.93	0.51
1:B:419:ARG:CG	6:B:2227:HOH:O	2.55	0.50
1:A:81:LYS:O	1:A:203:ARG:NH2	2.45	0.50
1:C:216:TYR:CE1	1:C:217:LEU:CD1	2.91	0.50
1:C:218:LYS:N	1:C:228:ASP:HB2	2.27	0.50
1:C:57:GLY:HA2	2:C:579:FAD:HM72	1.93	0.50
1:A:176:ARG:HD2	1:B:177:VAL:HG21	1.93	0.50
1:C:239:GLU:OE2	1:C:279:LYS:HD3	2.12	0.50
1:A:373:LEU:CD2	1:A:376:MET:HE3	2.24	0.49
1:B:306:PRO:CG	1:B:383:PRO:HB2	2.42	0.49
1:A:152:ASN:HD22	1:B:394:TRP:HE1	1.59	0.49
1:B:451:ALA:O	1:B:455:ILE:HG13	2.12	0.49
1:C:243:SER:HB2	1:C:244:PRO:CD	2.42	0.49
3:B:601:NAG:H4	3:B:602:NAG:C1	2.39	0.49
1:A:120:GLU:OE1	1:A:166:LYS:NZ	2.40	0.49
1:A:415:TYR:O	1:A:418:LEU:HB2	2.13	0.49
1:B:218:LYS:N	1:B:228:ASP:HB2	2.28	0.49
1:A:187:ALA:O	1:A:191:ASP:N	2.35	0.49
1:A:304:LYS:NZ	1:A:342:ALA:O	2.46	0.49
1:B:243:SER:HB2	1:B:244:PRO:HD2	1.94	0.49
1:B:247:VAL:HG11	1:B:262:VAL:HB	1.95	0.49
1:B:69:MET:HE3	1:B:73:TRP:CB	2.29	0.49
1:C:69:MET:HE3	6:C:2101:HOH:O	2.13	0.49
1:A:243:SER:CB	1:A:244:PRO:CD	2.91	0.49
1:B:143:MET:SD	1:B:147:ASN:ND2	2.86	0.49
3:B:601:NAG:O6	3:B:602:NAG:C1	2.60	0.49
1:C:119:VAL:HA	1:C:122:MET:CE	2.43	0.49
1:A:430:GLU:HG2	2:A:579:FAD:O3'	2.13	0.48
1:C:63:GLY:HA2	1:C:193:GLY:O	2.14	0.48
1:A:414:GLU:O	1:A:414:GLU:HG2	2.14	0.48
1:C:96:VAL:O	1:C:103:VAL:HA	2.13	0.48
1:C:112:ARG:NH2	1:C:115:LEU:CD1	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ILE:HG13	1:A:259:ALA:HB2	1.95	0.48
1:C:304:LYS:NZ	1:C:342:ALA:O	2.32	0.48
1:A:21:LYS:HB2	1:A:216:TYR:CE2	2.48	0.48
1:A:157:PRO:HG3	1:A:324:SER:HA	1.96	0.48
1:B:69:MET:CE	1:B:74:PRO:CD	2.84	0.48
1:C:173:GLU:OE1	1:C:294:ASP:OD2	2.32	0.48
1:A:69:MET:CE	1:A:74:PRO:CD	2.90	0.48
1:A:243:SER:HB2	1:A:244:PRO:HD2	1.95	0.48
1:B:69:MET:HE2	1:B:74:PRO:CD	2.24	0.48
1:C:218:LYS:O	1:C:227:VAL:N	2.40	0.48
1:A:450:SER:HA	1:A:453:ILE:HD12	1.96	0.48
1:C:64:VAL:O	1:C:65:ASN:HB2	2.13	0.48
1:C:69:MET:HE2	1:C:70:ASN:N	2.29	0.48
1:B:454:LEU:HD12	1:B:454:LEU:O	2.14	0.47
1:B:21:LYS:HB2	1:B:216:TYR:CE2	2.49	0.47
1:B:83:ARG:NH2	1:B:337:LYS:O	2.48	0.47
1:C:402:THR:CB	2:C:579:FAD:HM83	2.44	0.47
1:C:131:HIS:CD2	1:C:133:SER:HB3	2.50	0.47
1:C:69:MET:CE	1:C:73:TRP:HB3	2.44	0.47
1:A:431:HIS:CD2	6:A:2208:HOH:O	2.66	0.47
1:B:430:GLU:O	1:B:437:ASN:HA	2.14	0.47
1:A:95:ASN:HB3	1:A:319:PHE:HB3	1.96	0.47
1:C:366:LYS:HD2	1:C:385:ALA:HB3	1.97	0.47
1:B:241:LYS:HA	1:B:279:LYS:O	2.15	0.47
1:B:411:ASN:ND2	1:B:414:GLU:N	2.50	0.47
1:B:360:GLN:NE2	6:B:2189:HOH:O	2.48	0.47
1:A:70:ASN:O	1:A:74:PRO:HD3	2.15	0.47
1:A:238:ARG:NH1	1:A:252:GLU:OE2	2.47	0.46
1:A:305:PHE:HB3	1:A:306:PRO:HD2	1.96	0.46
1:C:26:ALA:HB2	1:C:455:ILE:HD13	1.96	0.46
1:C:438:GLY:O	2:C:579:FAD:H1'2	2.15	0.46
1:A:35:GLU:HB3	1:A:233:LEU:HD23	1.96	0.46
1:A:21:LYS:O	1:A:25:GLU:HG3	2.15	0.46
1:C:255:SER:HB2	1:C:257:TYR:CE1	2.50	0.46
1:A:305:PHE:HB3	1:A:306:PRO:CD	2.45	0.46
1:A:350:THR:HA	1:A:354:SER:OG	2.15	0.46
1:B:145:ARG:O	1:B:149:HIS:N	2.47	0.46
1:B:53:ASN:HB3	6:B:2099:HOH:O	2.15	0.46
1:C:187:ALA:HA	1:C:190:SER:OG	2.14	0.46
1:A:158:VAL:CG1	1:A:159:ASP:N	2.77	0.46
1:C:374:ARG:HD2	6:C:2194:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:601:NAG:O6	3:A:602:NAG:C1	2.63	0.46
1:B:218:LYS:H	1:B:228:ASP:HB2	1.79	0.46
1:A:291:TYR:CG	1:B:146:LEU:HA	2.51	0.46
1:C:285:TRP:CZ3	1:C:286:LYS:HE2	2.51	0.46
1:B:131:HIS:CD2	1:B:133:SER:OG	2.69	0.45
1:B:131:HIS:HD2	1:B:133:SER:CB	2.29	0.45
1:B:317:GLU:O	1:B:333:GLN:HA	2.15	0.45
1:A:99:GLU:HA	1:A:321:TYR:CE1	2.51	0.45
1:A:49:PHE:O	1:A:50:ALA:HB3	2.16	0.45
1:B:158:VAL:HG12	6:B:2072:HOH:O	2.16	0.45
1:B:246:GLY:HA2	1:B:424:ARG:HD3	1.99	0.45
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.65	0.45
1:A:292:GLN:OE1	6:A:2129:HOH:O	2.20	0.45
1:B:50:ALA:HB1	1:B:304:LYS:HD3	1.98	0.45
1:C:220:ASP:N	1:C:225:LYS:O	2.46	0.45
1:C:431:HIS:CD2	6:C:2231:HOH:O	2.69	0.45
1:C:430:GLU:O	1:C:437:ASN:HA	2.16	0.45
1:A:376:MET:C	1:A:378:PRO:HD3	2.36	0.45
1:C:250:LYS:HG2	1:C:256:VAL:HG22	1.97	0.45
1:C:8:ILE:HG13	1:C:259:ALA:HB2	1.99	0.45
1:A:300:LYS:HB3	1:A:346:LEU:HD11	1.98	0.45
1:B:141:LEU:HD22	1:B:176:ARG:HB3	1.97	0.45
1:B:307:ARG:HG2	1:B:383:PRO:HG3	1.99	0.45
1:B:411:ASN:HD21	1:B:414:GLU:H	1.58	0.44
1:B:411:ASN:HD21	1:B:414:GLU:HG3	1.82	0.44
1:A:303:LEU:O	1:A:344:VAL:HA	2.18	0.44
1:A:300:LYS:O	1:A:391:PRO:CD	2.65	0.44
1:A:256:VAL:HG12	1:A:257:TYR:N	2.32	0.44
1:A:69:MET:HE1	1:A:73:TRP:HB3	1.93	0.44
1:C:303:LEU:O	1:C:344:VAL:HA	2.18	0.44
1:C:198:PHE:CE2	1:C:338:GLN:HG2	2.52	0.44
1:C:342:ALA:O	1:C:343:ASN:HB2	2.18	0.44
1:C:439:TYR:HB3	1:C:441:HIS:CE1	2.53	0.44
1:A:73:TRP:N	1:A:74:PRO:CD	2.80	0.44
1:A:69:MET:HE2	1:A:74:PRO:CD	2.35	0.44
1:C:238:ARG:HD3	1:C:252:GLU:OE2	2.18	0.44
1:A:394:TRP:NE1	1:B:152:ASN:ND2	2.52	0.43
1:C:457:CYS:O	1:C:461:LYS:HA	2.19	0.43
1:A:452:GLU:HA	1:A:455:ILE:HD12	1.99	0.43
1:B:52:ILE:HG13	1:B:54:VAL:HG13	2.00	0.43
1:A:426:TYR:CE1	1:A:454:LEU:HD13	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:PHE:HB2	1:C:389:LEU:HB3	2.01	0.43
1:A:309:PHE:CD2	1:A:383:PRO:HD2	2.54	0.43
1:B:366:LYS:HD2	1:B:385:ALA:HB3	2.00	0.43
1:A:236:VAL:HB	1:A:252:GLU:HB2	2.01	0.43
1:A:73:TRP:HB3	1:A:74:PRO:HD3	1.99	0.43
1:B:293:PHE:CZ	1:B:406:TRP:HA	2.54	0.43
1:B:47:THR:O	1:B:53:ASN:HA	2.19	0.43
1:A:294:ASP:O	1:A:404:SER:HA	2.19	0.42
1:B:133:SER:O	1:B:411:ASN:HB2	2.19	0.42
1:C:243:SER:CB	1:C:244:PRO:CD	2.97	0.42
1:B:154:PRO:HB3	1:B:159:ASP:HB3	2.00	0.42
1:B:40:ILE:HD13	1:B:40:ILE:HG21	1.73	0.42
1:A:100:ASP:OD1	1:A:375:LYS:HE2	2.19	0.42
1:A:373:LEU:HA	1:A:376:MET:CE	2.49	0.42
1:A:370:MET:HG3	1:A:384:ASP:OD2	2.19	0.42
1:A:246:GLY:HA2	1:A:424:ARG:HD3	2.01	0.42
1:A:306:PRO:HG2	1:A:383:PRO:HB2	2.01	0.42
1:C:219:THR:CA	1:C:225:LYS:O	2.67	0.42
1:A:414:GLU:HG3	1:A:417:GLN:OE1	2.20	0.42
1:A:52:ILE:HG21	1:A:52:ILE:HD13	1.77	0.42
1:A:457:CYS:O	1:A:461:LYS:HA	2.20	0.42
1:C:118:SER:O	1:C:122:MET:HE2	2.20	0.42
1:A:302:PHE:HB2	1:A:389:LEU:HB3	2.02	0.42
1:A:64:VAL:CG1	1:A:65:ASN:N	2.82	0.42
1:A:180:LEU:HD12	1:A:184:VAL:HB	2.02	0.42
1:B:134:GLY:HA2	1:B:181:GLN:OE1	2.20	0.42
1:B:243:SER:O	1:B:424:ARG:HD2	2.20	0.42
1:C:294:ASP:HB2	1:C:405:ASN:O	2.19	0.42
1:B:243:SER:CB	1:B:244:PRO:CD	2.95	0.41
1:C:91:TYR:N	1:C:91:TYR:CD1	2.87	0.41
1:B:420:ALA:HA	1:B:421:PRO:HD3	1.90	0.41
1:C:48:ASN:HD21	1:C:51:GLY:HA2	1.85	0.41
1:C:69:MET:CE	1:C:69:MET:CA	2.97	0.41
1:A:302:PHE:O	1:A:388:ILE:HA	2.19	0.41
1:C:241:LYS:HA	1:C:279:LYS:O	2.20	0.41
1:A:220:ASP:OD1	1:A:223:SER:HB3	2.20	0.41
1:A:91:TYR:CG	1:A:315:GLY:HA3	2.55	0.41
1:B:319:PHE:CZ	1:B:332:TRP:HB3	2.55	0.41
1:C:370:MET:HE1	1:C:383:PRO:O	2.21	0.41
1:A:430:GLU:O	1:A:437:ASN:HA	2.20	0.41
1:A:400:LYS:HB3	1:B:151:PRO:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:VAL:CG1	6:B:2072:HOH:O	2.68	0.41
1:B:332:TRP:CZ3	1:B:347:VAL:HB	2.56	0.41
1:B:303:LEU:O	1:B:344:VAL:HA	2.20	0.41
1:B:430:GLU:OE1	1:B:438:GLY:N	2.51	0.41
1:A:271:LEU:HD23	1:A:271:LEU:HA	1.83	0.41
1:A:370:MET:CE	1:A:384:ASP:HA	2.51	0.41
1:B:75:ILE:HA	1:B:79:THR:HB	2.02	0.41
1:B:302:PHE:HB2	1:B:389:LEU:HB3	2.03	0.41
1:C:66:GLY:HA3	1:C:192:PHE:C	2.41	0.41
1:C:6:ARG:HG3	1:C:6:ARG:NH1	2.29	0.41
1:B:148:GLU:O	1:B:149:HIS:HB2	2.21	0.41
1:B:312:GLU:OE2	6:B:2148:HOH:O	2.22	0.41
1:C:21:LYS:O	1:C:25:GLU:HG3	2.20	0.41
1:C:23:LEU:HB3	1:C:28:ILE:HB	2.01	0.41
1:A:235:LYS:HA	1:A:235:LYS:HD3	1.74	0.41
1:B:216:TYR:CD1	1:B:217:LEU:CD1	3.00	0.41
1:B:8:ILE:O	1:B:262:VAL:HA	2.21	0.41
1:B:411:ASN:C	1:B:411:ASN:HD22	2.24	0.41
1:C:213:ALA:O	1:C:217:LEU:HB2	2.21	0.41
1:A:273:SER:O	1:A:274:ASP:CB	2.57	0.40
1:A:69:MET:HE3	1:A:73:TRP:CB	2.37	0.40
1:A:360:GLN:NE2	6:A:2173:HOH:O	2.54	0.40
1:B:220:ASP:CB	1:B:223:SER:OG	2.61	0.40
1:B:228:ASP:OD1	1:B:229:PRO:HD2	2.22	0.40
1:C:119:VAL:HA	1:C:122:MET:HE2	2.03	0.40
1:B:26:ALA:CB	1:B:455:ILE:HD13	2.50	0.40
1:B:57:GLY:HA2	2:B:579:FAD:C7M	2.51	0.40
1:C:154:PRO:HB3	1:C:159:ASP:HB3	2.03	0.40
1:C:50:ALA:HB1	1:C:304:LYS:HD3	2.03	0.40
1:C:317:GLU:O	1:C:333:GLN:HA	2.22	0.40
1:A:91:TYR:N	1:A:91:TYR:CD1	2.89	0.40
1:B:381:ASP:O	1:B:383:PRO:HD3	2.21	0.40
1:B:370:MET:HG3	1:B:384:ASP:OD2	2.21	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	457/472 (97%)	437 (96%)	19 (4%)	1 (0%)	51	52
1	B	460/472 (98%)	444 (96%)	16 (4%)	0	100	100
1	C	460/472 (98%)	442 (96%)	18 (4%)	0	100	100
All	All	1377/1416 (97%)	1323 (96%)	53 (4%)	1 (0%)	55	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	GLY

### 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	394/404 (98%)	381 (97%)	13 (3%)	43	45
1	B	397/404 (98%)	384 (97%)	13 (3%)	43	45
1	C	397/404 (98%)	391 (98%)	6 (2%)	70	76
All	All	1188/1212 (98%)	1156 (97%)	32 (3%)	50	54

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

Mol	Chain	Res	Type
1	A	23	LEU
1	A	28	ILE

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Mol	Chain	Res	Type
1	A	52	ILE
1	A	59	ASN
1	A	136	ASP
1	A	168	ASP
1	A	186	LEU
1	A	190	SER
1	A	205	TYR
1	A	215	GLN
1	A	217	LEU
1	A	282	LEU
1	A	386	THR
1	B	23	LEU
1	B	59	ASN
1	B	105	ASP
1	B	115	LEU
1	B	154	PRO
1	B	157	PRO
1	B	158	VAL
1	B	168	ASP
1	B	205	TYR
1	B	217	LEU
1	B	411	ASN
1	B	430	GLU
1	B	454	LEU
1	C	59	ASN
1	C	127	SER
1	C	205	TYR
1	C	217	LEU
1	C	221	ASP
1	C	282	LEU

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	152	ASN
1	A	292	GLN
1	A	360	GLN
1	A	431	HIS
1	B	131	HIS
1	B	152	ASN
1	B	360	GLN
1	B	411	ASN

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Mol	Chain	Res	Type
1	B	431	HIS
1	B	466	HIS
1	C	48	ASN
1	C	131	HIS
1	C	152	ASN
1	C	360	GLN
1	C	431	HIS

### 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 ⓘ

4 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$
4	NAG	C	601	1,3,4	14,14,15	1.10	1 (7%)	15,19,21	2.07	5 (33%)
4	FCA	C	603	4	9,10,11	1.44	1 (11%)	13,14,16	1.91	4 (30%)
5	MAN	C	604	3,5	11,11,12	0.67	0	13,15,17	3.51	3 (23%)
5	MAN	C	605	5	11,11,12	0.54	0	13,15,17	1.21	2 (15%)

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
4	NAG	C	601	1,3,4	-	0/6/23/26	0/1/1/1
4	FCA	C	603	4	-	0/0/17/20	0/1/1/1
5	MAN	C	604	3,5	1/1/4/5	0/2/19/22	0/1/1/1
5	MAN	C	605	5	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	FCA	C2-C3	-3.37	1.48	1.52
4	C	601	NAG	C1-C2	-2.52	1.49	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	NAG	C1-C2-N2	-4.70	102.45	110.49
4	C	603	FCA	C3-C4-C5	-3.58	104.06	109.68
4	C	601	NAG	C8-C7-N2	-2.85	110.95	116.11
5	C	605	MAN	C2-C3-C4	-2.69	106.18	110.88
4	C	603	FCA	C2-C3-C4	-2.40	106.69	110.88
4	C	601	NAG	O5-C1-C2	-2.23	108.36	111.47
5	C	604	MAN	O5-C1-C2	2.09	114.07	110.79
4	C	601	NAG	C4-C3-C2	2.35	114.46	111.02
4	C	603	FCA	C1-O5-C5	2.43	117.77	112.39
5	C	604	MAN	O3-C3-C2	2.46	114.50	110.02
5	C	605	MAN	O2-C2-C3	2.80	115.67	110.17
4	C	603	FCA	C1-C2-C3	3.28	113.81	109.65
4	C	601	NAG	C1-O5-C5	3.77	117.37	112.17
5	C	604	MAN	O2-C2-C3	11.83	133.41	110.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	604	MAN	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	NAG	6	0
4	C	603	FCA	2	0

## 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	579	-	51,58,58	0.95	2 (3%)	54,89,89	2.42	14 (25%)
3	NAG	A	601	1,3	14,14,15	0.90	0	15,19,21	1.75	5 (33%)
3	NAG	A	602	3	14,14,15	0.92	1 (7%)	15,19,21	1.44	2 (13%)
2	FAD	B	579	-	51,58,58	0.87	2 (3%)	54,89,89	1.99	11 (20%)
3	NAG	B	601	1,3	14,14,15	1.14	2 (14%)	15,19,21	1.91	4 (26%)
3	NAG	B	602	3	14,14,15	0.95	1 (7%)	15,19,21	1.64	3 (20%)
2	FAD	C	579	-	51,58,58	1.09	4 (7%)	54,89,89	2.23	10 (18%)
3	NAG	C	602	5,4	14,14,15	1.18	2 (14%)	15,19,21	1.71	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
2	FAD	A	579	-	-	0/28/50/50	0/6/6/6
3	NAG	A	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	602	3	-	0/6/23/26	0/1/1/1
2	FAD	B	579	-	-	0/28/50/50	0/6/6/6
3	NAG	B	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	602	3	-	0/6/23/26	0/1/1/1
2	FAD	C	579	-	-	0/28/50/50	0/6/6/6
3	NAG	C	602	5,4	-	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	NAG	O5-C1	-3.28	1.38	1.43
2	B	579	FAD	C2-N1	-2.74	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	579	FAD	C2-N1	-2.67	1.32	1.38
2	A	579	FAD	C2-N1	-2.62	1.33	1.38
3	B	601	NAG	C1-C2	-2.58	1.48	1.52
3	B	602	NAG	O5-C1	-2.57	1.39	1.43
3	C	602	NAG	C1-C2	-2.41	1.49	1.52
3	B	601	NAG	O5-C1	-2.38	1.39	1.43
3	A	602	NAG	O5-C1	-2.30	1.39	1.43
2	C	579	FAD	C10-N1	2.56	1.36	1.33
2	C	579	FAD	C4X-N5	2.68	1.37	1.33
2	C	579	FAD	C4-N3	3.20	1.38	1.33
2	B	579	FAD	C4-N3	3.21	1.38	1.33
2	A	579	FAD	C4-N3	3.99	1.40	1.33

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	579	FAD	C4X-C10-N10	-7.35	115.42	120.52
2	A	579	FAD	C4X-C4-N3	-6.48	114.26	123.48
2	A	579	FAD	C4X-C10-N10	-5.33	116.82	120.52
2	C	579	FAD	C4-C4X-C10	-4.91	115.99	119.96
2	B	579	FAD	C4X-C4-N3	-4.46	117.14	123.48
2	C	579	FAD	C4X-C4-N3	-4.03	117.75	123.48
3	B	601	NAG	C2-N2-C7	-4.00	117.11	122.94
3	C	602	NAG	O5-C1-C2	-3.73	106.29	111.47
3	B	602	NAG	C2-N2-C7	-3.57	117.73	122.94
2	B	579	FAD	C4X-C10-N10	-3.56	118.05	120.52
2	A	579	FAD	C9A-C5X-N5	-3.38	117.21	122.24
3	A	602	NAG	C1-C2-N2	-3.34	104.78	110.49
2	B	579	FAD	C4-C4X-C10	-3.28	117.31	119.96
3	A	601	NAG	C1-C2-N2	-3.09	105.21	110.49
3	A	601	NAG	C8-C7-N2	-2.80	111.05	116.11
2	A	579	FAD	C10-C4X-N5	-2.75	117.43	120.59
2	B	579	FAD	O2B-C2B-C1B	-2.58	103.55	111.61
3	B	602	NAG	C1-C2-N2	-2.49	106.24	110.49
3	B	601	NAG	C1-C2-N2	-2.40	106.38	110.49
2	B	579	FAD	O3'-C3'-C4'	-2.33	103.05	108.82
2	A	579	FAD	C4-C4X-C10	-2.29	118.11	119.96
2	A	579	FAD	C8M-C8-C9	-2.25	114.71	120.34
3	A	602	NAG	C2-N2-C7	-2.09	119.89	122.94
2	A	579	FAD	C4B-O4B-C1B	-2.05	107.59	109.77
2	B	579	FAD	C4X-N5-C5X	-2.01	114.64	116.76
3	C	602	NAG	O3-C3-C2	-2.01	105.08	109.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	579	FAD	O2A-PA-O1A	2.05	122.87	112.28
2	C	579	FAD	C2B-C3B-C4B	2.06	106.63	102.62
2	C	579	FAD	O2P-P-O1P	2.10	123.13	112.28
2	B	579	FAD	C4A-C5A-N7A	2.10	111.44	109.41
2	A	579	FAD	N3A-C2A-N1A	2.14	130.72	128.86
3	C	602	NAG	C3-C4-C5	2.21	114.11	110.22
2	A	579	FAD	O2P-P-O1P	2.24	123.87	112.28
3	A	601	NAG	O3-C3-C4	2.34	115.45	110.36
2	A	579	FAD	O2A-PA-O1A	2.35	124.46	112.28
3	A	601	NAG	C6-C5-C4	2.37	118.54	113.00
2	C	579	FAD	C4A-C5A-N7A	2.50	111.82	109.41
3	B	601	NAG	O3-C3-C2	2.52	114.79	109.39
2	C	579	FAD	C1'-N10-C9A	2.59	120.72	118.35
2	C	579	FAD	O2A-PA-O1A	2.82	126.86	112.28
2	A	579	FAD	O4'-C4'-C3'	2.84	116.14	109.09
2	A	579	FAD	C6-C5X-C9A	2.89	122.75	119.00
3	B	602	NAG	C1-O5-C5	3.04	116.36	112.17
3	A	601	NAG	C1-O5-C5	3.08	116.41	112.17
2	B	579	FAD	C4-C4X-N5	3.24	122.23	118.68
2	B	579	FAD	C1'-N10-C9A	3.45	121.51	118.35
2	C	579	FAD	C4-C4X-N5	3.49	122.51	118.68
3	B	601	NAG	C1-O5-C5	3.69	117.25	112.17
2	A	579	FAD	C1'-N10-C9A	6.86	124.63	118.35
2	B	579	FAD	C4-N3-C2	8.88	122.93	115.16
2	A	579	FAD	C4-N3-C2	9.63	123.58	115.16
2	C	579	FAD	C4-N3-C2	9.76	123.70	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	579	FAD	2	0
3	A	601	NAG	3	0
3	A	602	NAG	3	0
2	B	579	FAD	2	0
3	B	601	NAG	4	0
3	B	602	NAG	4	0
2	C	579	FAD	5	0
3	C	602	NAG	4	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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.