Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:47 PM 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

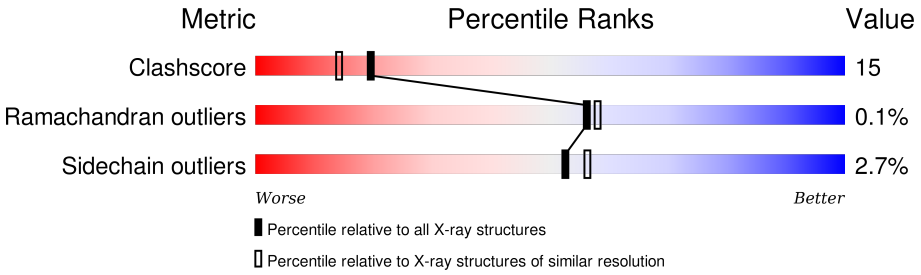
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (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 >=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 <=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	66% 29%
1	B	472	70% 26%
1	C	472	71% 26%

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

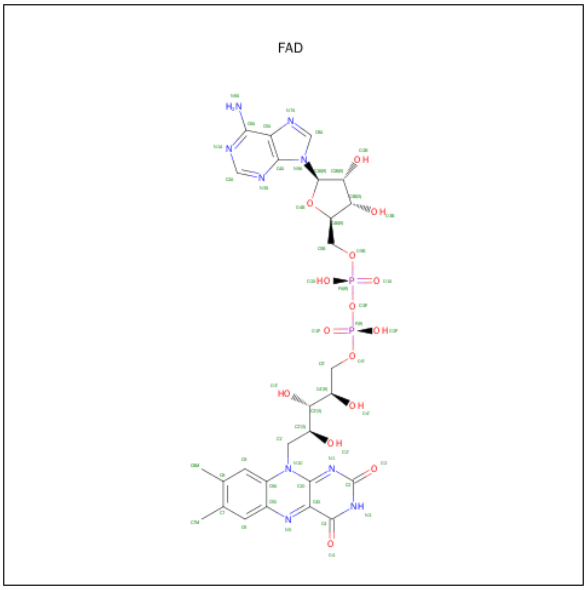
There are 6 unique types of molecules in this entry. The entry contains 12113 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

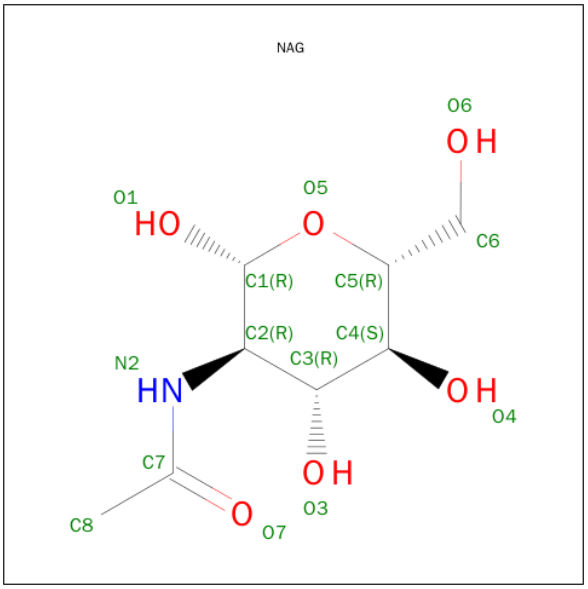
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	55	0	0
			3684	2353	621	696	14			
1	B	462	Total	C	N	O	S	61	0	0
			3715	2374	627	700	14			
1	C	462	Total	C	N	O	S	50	0	0
			3715	2374	627	700	14			

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

- 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 24 14 1 9	0	0

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

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

- Molecule 6 is water.

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

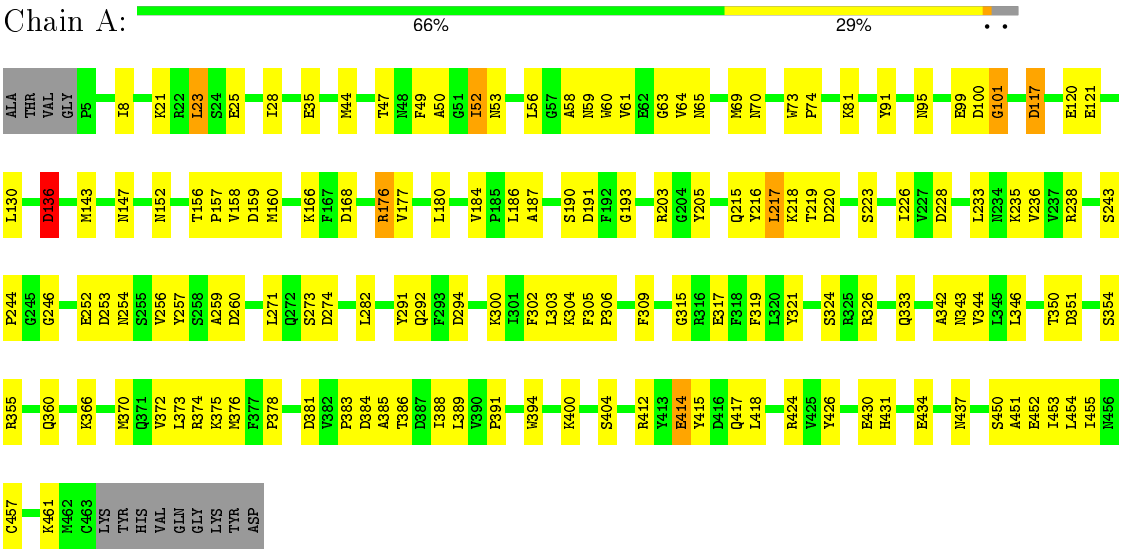
3 Residue-property plots (i)

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.

Note EDS was not executed.

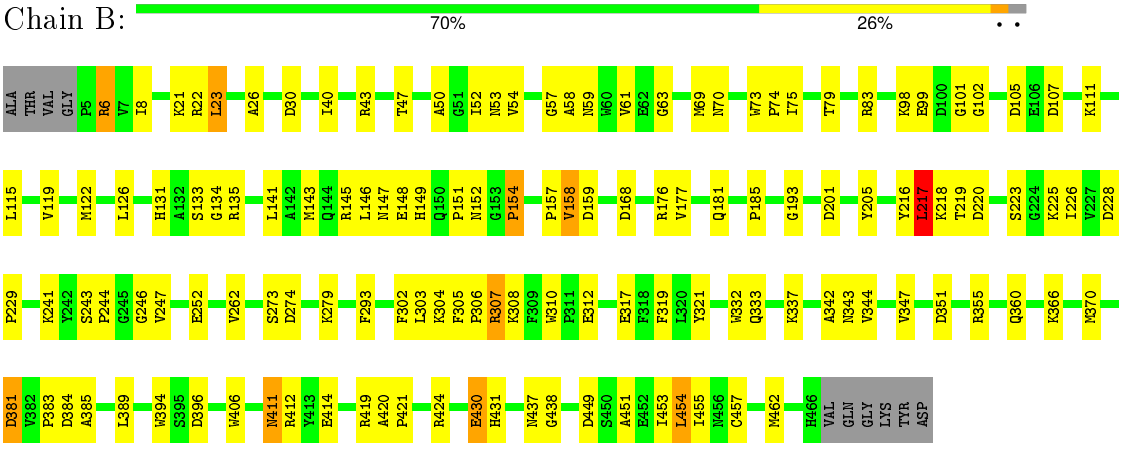
- Molecule 1: POLYAMINE OXIDASE

Chain A:



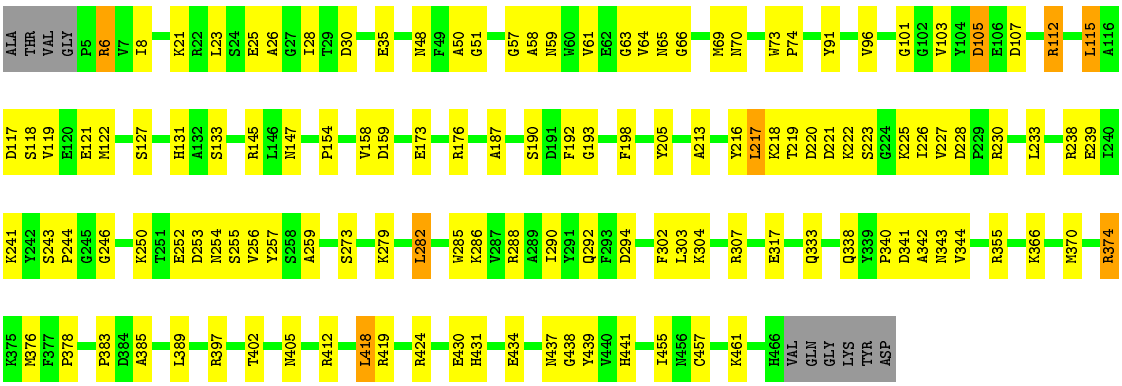
- Molecule 1: POLYAMINE OXIDASE

Chain B:



- Molecule 1: POLYAMINE OXIDASE

Chain C:


ALA THR VAL GLY P5 R6 V7 I8 K21 R22 L23 S24 E25 A26 G27 I28 T29 D30 E35 N48 F49 A50 G51 G57 A58 N59 W60 V61 F62 G63 V64 N65 G66 M69 N70 W73 P74 Y91 V96 G101 G102 Y103 Y104 D105 E106 D107 R112 L115 A116
D117 S118 V119 E120 E121 M122 S127 H131 A132 S133 R145 L146 N147 P154 V158 D159 E173 R176 A187 S190 D191 F192 G193 F198 Y205 A213 Y216 L217 K218 T219 D220 D221 K222 S223 G224 K225 I226 V227 D228 P229 R230 L233 R238 E239 I240
K241 Y242 S243 P244 G245 G246 K250 T251 E252 D253 N254 S255 V256 Y257 S258 A259 S273 K279 L282 W285 K286 V287 R288 A289 I290 Y291 Q292 F293 D294 F302 L303 K304 R307 E317 Q333 Q338 Y339 P340 D341 A342 N343 V344 R355 K366 M370 R374
K375 M376 F377 P378 P383 D384 A385 I389 R397 T402 N405 R412 L418 R419 R424 E430 H431 E434 N437 G438 Y439 V440 H441 I455 N456 C457 K461 H466 VAL GLN GLY LYS TYR ASP

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	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^2)	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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (i)

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:C:112:ARG:HD3	1:C:159:ASP:OD1	1.77	0.84
1:B:119:VAL:HA	1:B:122:MET:HE3	1.57	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
4:C:601:NAG:O4	3:C:602:NAG:C2	2.35	0.74
1:A:69:MET:CE	1:A:74:PRO:HD3	2.16	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:C:131:HIS:HD2	1:C:133:SER:OG	1.76	0.69
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: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
4:C:601:NAG:H4	3:C:602:NAG:C1	2.28	0.64
1:A:158:VAL:HG13	1:A:159:ASP:N	2.13	0.64
1:C:69:MET:CE	1:C:70:ASN:H	2.11	0.64
1:B:412:ARG:HG3	6:B:2215:HOH:O	1.96	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:C:412:ARG:NH1	1:C:434:GLU:OE2	2.33	0.59
1:A:177:VAL:HG11	1:B:176:ARG:HD2	1.83	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:C:69:MET:HE3	1:C:69:MET:CA	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:SER:O	1:B:274:ASP:HB2	2.03	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:C:131:HIS:HD2	1:C:133:SER:N	2.03	0.57
1:B:243:SER:HB2	1:B:244:PRO:CD	2.35	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:C:219:THR:HA	1:C:225:LYS:O	2.07	0.54
1:B:454:LEU:C	1:B:454:LEU:HD12	2.28	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:C:158:VAL:HG12	6:C:2073:HOH:O	2.06	0.53
1:B:306:PRO:HG3	1:B:383:PRO:HB2	1.90	0.53
1:B:69:MET:HE1	1:B:73:TRP:HB3	1.84	0.53
1:A:216:TYR:CE1	1:A:217:LEU:HD13	2.43	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:B:131:HIS:HD2	1:B:133:SER:OG	1.93	0.52
1:A:156:THR:O	1:A:160:MET:HG3	2.09	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:C:21:LYS:HB2	1:C:216:TYR:CE2	2.45	0.52
1:B:98:LYS:HG3	1:B:102:GLY:O	2.10	0.52
1:C:112:ARG:NH2	1:C:115:LEU:HD11	2.24	0.52
1:C:376:MET:C	1:C:378:PRO:HD3	2.30	0.51
1:C:246:GLY:HA2	1:C:424:ARG:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:GLY:HA2	2:C:579:FAD:C7M	2.41	0.51
1:B:99:GLU:HA	1:B:321:TYR:CE1	2.46	0.51
1:A:253:ASP:O	1:A:254:ASN:HB2	2.11	0.51
3:A:601:NAG:H4	3:A:602:NAG:C1	2.39	0.51
1:A:317:GLU:O	1:A:333:GLN:HA	2.10	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:C:216:TYR:CE1	1:C:217:LEU:CD1	2.91	0.50
1:A:81:LYS:O	1:A:203:ARG:NH2	2.45	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:A:152:ASN:HD22	1:B:394:TRP:HE1	1.59	0.49
1:B:306:PRO:CG	1:B:383:PRO:HB2	2.42	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: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:120:GLU:OE1	1:A:166:LYS:NZ	2.40	0.49
1:A:304:LYS:NZ	1:A:342:ALA:O	2.46	0.49
1:A:187:ALA:O	1:A:191:ASP:N	2.35	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: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
3:B:601:NAG:O6	3:B:602:NAG:C1	2.60	0.49
1:A:243:SER:CB	1:A:244:PRO:CD	2.91	0.49
1:C:119:VAL:HA	1:C:122:MET:CE	2.43	0.49
1:B:143:MET:SD	1:B:147:ASN:ND2	2.86	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:C:112:ARG:NH2	1:C:115:LEU:CD1	2.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:LYS:NZ	1:C:342:ALA:O	2.32	0.48
1:A:8:ILE:HG13	1:A:259:ALA:HB2	1.95	0.48
1:B:69:MET:CE	1:B:74:PRO:CD	2.84	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: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:B:69:MET:HE2	1:B:74:PRO:CD	2.24	0.48
1:A:243:SER:HB2	1:A:244:PRO:HD2	1.95	0.48
1:C:218:LYS:O	1:C:227:VAL:N	2.40	0.48
1:C:69:MET:HE2	1:C:70:ASN:N	2.29	0.48
1:C:64:VAL:O	1:C:65:ASN:HB2	2.13	0.48
1:A:450:SER:HA	1:A:453:ILE:HD12	1.96	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:C:402:THR:CB	2:C:579:FAD:HM83	2.44	0.47
1:B:83:ARG:NH2	1:B:337:LYS:O	2.48	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:B:411:ASN:ND2	1:B:414:GLU:N	2.50	0.47
1:C:366:LYS:HD2	1:C:385:ALA:HB3	1.97	0.47
1:A:95:ASN:HB3	1:A:319:PHE:HB3	1.96	0.47
1:B:241:LYS:HA	1:B:279:LYS:O	2.15	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:C:438:GLY:O	2:C:579:FAD:H1'2	2.15	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:A:21:LYS:O	1:A:25:GLU:HG3	2.15	0.46
1:A:35:GLU:HB3	1:A:233:LEU:HD23	1.96	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:C:187:ALA:HA	1:C:190:SER:OG	2.14	0.46
1:B:53:ASN:HB3	6:B:2099:HOH:O	2.15	0.46
1:B:145:ARG:O	1:B:149:HIS:N	2.47	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:49:PHE:O	1:A:50:ALA:HB3	2.16	0.45
1:B:246:GLY:HA2	1:B:424:ARG:HD3	1.99	0.45
1:A:99:GLU:HA	1:A:321:TYR:CE1	2.51	0.45
1:B:158:VAL:HG12	6:B:2072:HOH:O	2.16	0.45
1:C:220:ASP:N	1:C:225:LYS:O	2.46	0.45
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.65	0.45
1:C:431:HIS:CD2	6:C:2231:HOH:O	2.69	0.45
1:B:50:ALA:HB1	1:B:304:LYS:HD3	1.98	0.45
1:C:430:GLU:O	1:C:437:ASN:HA	2.16	0.45
1:A:292:GLN:OE1	6:A:2129:HOH:O	2.20	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:342:ALA:O	1:C:343:ASN:HB2	2.18	0.44
1:C:198:PHE:CE2	1:C:338:GLN:HG2	2.52	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:B:52:ILE:HG13	1:B:54:VAL:HG13	2.00	0.43
1:A:452:GLU:HA	1:A:455:ILE:HD12	1.99	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:47:THR:O	1:B:53:ASN:HA	2.19	0.43
1:B:293:PHE:CZ	1:B:406:TRP:HA	2.54	0.43
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:A:294:ASP:O	1:A:404:SER:HA	2.19	0.42
1:B:40:ILE:HD13	1:B:40:ILE:HG21	1.73	0.42
1:B:154:PRO:HB3	1:B:159:ASP:HB3	2.00	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:100:ASP:OD1	1:A:375:LYS:HE2	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:52:ILE:HG21	1:A:52:ILE:HD13	1.77	0.42
1:A:414:GLU:HG3	1:A:417:GLN:OE1	2.20	0.42
1:C:118:SER:O	1:C:122:MET:HE2	2.20	0.42
1:A:457:CYS:O	1:A:461:LYS:HA	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: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: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: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:C:69:MET:CE	1:C:69:MET:CA	2.97	0.41
1:C:48:ASN:HD21	1:C:51:GLY:HA2	1.85	0.41
1:B:420:ALA:HA	1:B:421:PRO:HD3	1.90	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:C:370:MET:HE1	1:C:383:PRO:O	2.21	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:A:430:GLU:O	1:A:437:ASN:HA	2.20	0.41
1:B:430:GLU:OE1	1:B:438:GLY:N	2.51	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:A:400:LYS:HB3	1:B:151:PRO:HG3	2.01	0.41
1:B:303:LEU:O	1:B:344:VAL:HA	2.20	0.41
1:A:370:MET:CE	1:A:384:ASP:HA	2.51	0.41
1:A:271:LEU:HD23	1:A:271:LEU:HA	1.83	0.41
1:B:75:ILE:HA	1:B:79:THR:HB	2.02	0.41
1:C:6:ARG:HG3	1:C:6:ARG:NH1	2.29	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:21:LYS:O	1:C:25:GLU:HG3	2.20	0.41
1:B:148:GLU:O	1:B:149:HIS:HB2	2.21	0.41
1:C:23:LEU:HB3	1:C:28:ILE:HB	2.01	0.41
1:B:312:GLU:OE2	6:B:2148:HOH:O	2.22	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: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:A:235:LYS:HA	1:A:235:LYS:HD3	1.74	0.41
1:A:69:MET:HE3	1:A:73:TRP:CB	2.37	0.40
1:A:273:SER:O	1:A:274:ASP:CB	2.57	0.40
1:B:220:ASP:CB	1:B:223:SER:OG	2.61	0.40
1:C:119:VAL:HA	1:C:122:MET:HE2	2.03	0.40
1:B:228:ASP:OD1	1:B:229:PRO:HD2	2.22	0.40
1:A:360:GLN:NE2	6:A:2173:HOH:O	2.54	0.40
1:C:154:PRO:HB3	1:C:159:ASP:HB3	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: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:B:381:ASP:O	1:B:383:PRO:HD3	2.21	0.40
1:A:91:TYR:N	1:A:91:TYR:CD1	2.89	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	457/472 (97%)	437 (96%)	19 (4%)	1 (0%)	52	53
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%)	56	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	394/404 (98%)	381 (97%)	13 (3%)	45	47
1	B	397/404 (98%)	384 (97%)	13 (3%)	45	47
1	C	397/404 (98%)	391 (98%)	6 (2%)	72	78
All	All	1188/1212 (98%)	1156 (97%)	32 (3%)	52	56

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	1.08	1 (7%)	15,19,21	1.58	3 (20%)
4	FCA	C	603	4	10,10,11	1.33	1 (10%)	14,14,16	2.00	4 (28%)
5	MAN	C	604	3,5	11,11,12	0.66	0	14,15,17	3.34	2 (14%)
5	MAN	C	605	5	11,11,12	0.53	0	14,15,17	1.19	2 (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
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	-3.30	1.48	1.52
4	C	601	NAG	C1-C2	-2.53	1.49	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	603	FCA	C3-C4-C5	-3.36	104.06	109.72
5	C	605	MAN	C2-C3-C4	-2.86	106.18	111.04
4	C	601	NAG	C8-C7-N2	-2.69	110.95	116.11
4	C	603	FCA	C2-C3-C4	-2.56	106.69	111.04
4	C	601	NAG	C4-C3-C2	2.08	114.46	111.23
5	C	604	MAN	O3-C3-C2	2.49	114.50	110.00
5	C	605	MAN	O2-C2-C3	2.76	115.67	110.12
4	C	603	FCA	C1-O5-C5	3.49	117.77	112.38
4	C	603	FCA	C1-C2-C3	3.61	113.81	109.54
4	C	601	NAG	C1-O5-C5	4.03	117.37	112.25
5	C	604	MAN	O2-C2-C3	11.58	133.41	110.12

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 (i)

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	-	48,58,58	1.02	2 (4%)	54,89,89	2.40	13 (24%)
3	NAG	A	601	1,3	14,14,15	0.88	0	15,19,21	1.71	5 (33%)
3	NAG	A	602	3	14,14,15	0.90	1 (7%)	15,19,21	1.09	1 (6%)
2	FAD	B	579	-	48,58,58	0.79	1 (2%)	54,89,89	2.03	9 (16%)
3	NAG	B	601	1,3	14,14,15	1.12	2 (14%)	15,19,21	2.06	4 (26%)
3	NAG	B	602	3	14,14,15	0.94	1 (7%)	15,19,21	1.87	3 (20%)
2	FAD	C	579	-	48,58,58	0.95	2 (4%)	54,89,89	2.37	8 (14%)
3	NAG	C	602	5,4	14,14,15	1.17	2 (14%)	15,19,21	1.66	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	-	-	0/30/50/50	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	-	-	0/30/50/50	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	-	-	0/30/50/50	0/6/6/6
3	NAG	C	602	5,4	-	0/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	579	FAD	C10-N10	-3.37	1.35	1.39
3	C	602	NAG	O5-C1	-3.21	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	NAG	C1-C2	-2.59	1.48	1.52
3	B	602	NAG	O5-C1	-2.52	1.39	1.43
3	C	602	NAG	C1-C2	-2.42	1.49	1.52
3	B	601	NAG	O5-C1	-2.33	1.39	1.43
3	A	602	NAG	O5-C1	-2.25	1.39	1.43
2	C	579	FAD	C4X-N5	2.45	1.37	1.33
2	C	579	FAD	C4-N3	3.09	1.38	1.33
2	B	579	FAD	C4-N3	3.10	1.38	1.33
2	A	579	FAD	C4-N3	3.86	1.40	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	579	FAD	C4X-C10-N10	-8.66	115.42	120.52
2	A	579	FAD	C4X-C4-N3	-6.82	114.26	123.59
2	A	579	FAD	C4X-C10-N10	-6.27	116.82	120.52
2	C	579	FAD	C4-C4X-C10	-6.17	115.99	119.94
2	B	579	FAD	C4X-C4-N3	-4.72	117.14	123.59
3	B	601	NAG	C2-N2-C7	-4.62	117.11	123.04
2	C	579	FAD	C4X-C4-N3	-4.27	117.75	123.59
2	B	579	FAD	C4X-C10-N10	-4.20	118.05	120.52
3	B	602	NAG	C2-N2-C7	-4.13	117.73	123.04
2	B	579	FAD	C4-C4X-C10	-4.11	117.31	119.94
2	A	579	FAD	C9A-C5X-N5	-3.48	117.21	122.36
3	C	602	NAG	O5-C5-C6	-3.41	99.96	107.35
3	B	602	NAG	O5-C5-C6	-3.31	100.18	107.35
2	A	579	FAD	C4-C4X-C10	-2.86	118.11	119.94
3	A	601	NAG	C8-C7-N2	-2.64	111.05	116.11
3	B	601	NAG	O5-C5-C6	-2.60	101.72	107.35
3	A	602	NAG	C2-N2-C7	-2.45	119.89	123.04
3	A	601	NAG	O5-C5-C6	-2.44	102.07	107.35
2	A	579	FAD	O3P-P-O5'	-2.38	96.61	102.94
2	B	579	FAD	O3'-C3'-C4'	-2.26	103.05	108.75
2	C	579	FAD	P-O3P-PA	-2.24	126.43	132.73
2	A	579	FAD	C8M-C8-C9	-2.05	114.71	120.28
3	C	602	NAG	O3-C3-C2	-2.03	105.08	109.11
2	A	579	FAD	O2P-P-O1P	2.09	123.87	112.53
2	B	579	FAD	C4A-C5A-N7A	2.13	111.44	109.48
2	A	579	FAD	O2A-PA-O1A	2.20	124.46	112.53
3	A	601	NAG	C6-C5-C4	2.24	118.54	113.02
3	C	602	NAG	C3-C4-C5	2.25	114.11	110.20
3	A	601	NAG	O3-C3-C4	2.27	115.45	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	579	FAD	C1'-N10-C9A	2.36	121.51	118.86
2	A	579	FAD	N3A-C2A-N1A	2.38	130.72	128.89
2	C	579	FAD	C4A-C5A-N7A	2.55	111.82	109.48
2	C	579	FAD	O2A-PA-O1A	2.64	126.86	112.53
2	A	579	FAD	O4'-C4'-C3'	2.83	116.14	109.02
2	A	579	FAD	C6-C5X-C9A	2.86	122.75	118.98
3	B	601	NAG	O3-C3-C2	2.87	114.79	109.11
2	B	579	FAD	C4-C4X-N5	2.89	122.23	118.72
2	C	579	FAD	C4-C4X-N5	3.12	122.51	118.72
2	B	579	FAD	C2B-C1B-N9A	3.22	119.22	114.29
3	B	602	NAG	C1-O5-C5	3.24	116.36	112.25
3	A	601	NAG	C1-O5-C5	3.28	116.41	112.25
3	B	601	NAG	C1-O5-C5	3.94	117.25	112.25
2	A	579	FAD	C1'-N10-C9A	5.14	124.63	118.86
2	B	579	FAD	C4-N3-C2	8.88	122.93	115.25
2	A	579	FAD	C4-N3-C2	9.64	123.58	115.25
2	C	579	FAD	C4-N3-C2	9.77	123.70	115.25

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

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.