



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:53 AM GMT

PDB ID : 3JSX  
Title : X-ray Crystal structure of NAD(P)H: Quinone Oxidoreductase-1 (NQO1)  
bound to the coumarin-based inhibitor AS1  
Authors : Dunstan, M.S.; Levy, C.; Leys, D.  
Deposited on : 2009-09-11  
Resolution : 2.45 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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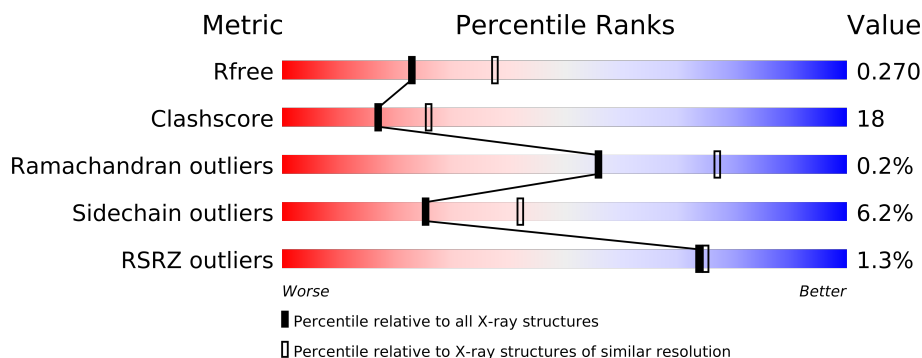
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 2.45 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	3566 (2.50-2.42)
Clashscore	79885	4471 (2.50-2.42)
Ramachandran outliers	78287	4383 (2.50-2.42)
Sidechain outliers	78261	4385 (2.50-2.42)
RSRZ outliers	66119	3568 (2.50-2.42)

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	273	
1	B	273	
1	C	273	
1	D	273	
1	E	273	
1	F	273	
1	G	273	
1	H	273	

## 2 Entry composition

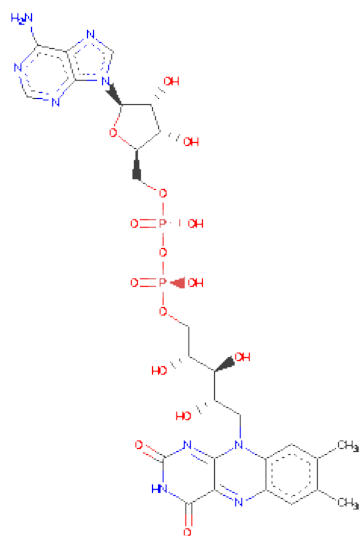
There are 4 unique types of molecules in this entry. The entry contains 18234 atoms, of which 0 are hydrogen and 0 are deuterium.

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 (with D amino acids) called NAD(P)H dehydrogenase [quinone] 1.

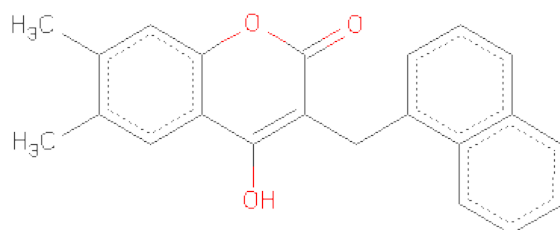
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total 2147	C 1397	N 358	O 385	S 7	0	0	0
1	B	270	Total 2147	C 1397	N 358	O 385	S 7	0	0	0
1	C	270	Total 2147	C 1397	N 358	O 385	S 7	0	0	0
1	D	270	Total 2147	C 1397	N 358	O 385	S 7	0	0	0
1	E	270	Total 2147	C 1397	N 358	O 385	S 7	0	0	0
1	F	270	Total 2147	C 1397	N 358	O 385	S 7	0	0	0
1	G	270	Total 2147	C 1397	N 358	O 385	S 7	0	0	0
1	H	270	Total 2147	C 1397	N 358	O 385	S 7	0	0	0

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



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

- Molecule 3 is 4-HYDROXY-6,7-DIMETHYL-3-(NAPHTHALEN-1-YLMETHYL)-2H-CHROMEN-2-ONE (three-letter code: CC2) (formula: C<sub>22</sub>H<sub>18</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			25	22	3		
3	B	1	Total	C	O	0	0
			25	22	3		
3	C	1	Total	C	O	0	0
			25	22	3		
3	D	1	Total	C	O	0	0
			25	22	3		
3	E	1	Total	C	O	0	0
			25	22	3		
3	F	1	Total	C	O	0	0
			25	22	3		
3	G	1	Total	C	O	0	0
			25	22	3		
3	H	1	Total	C	O	0	0
			25	22	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total	O	0	0
			66	66		
4	B	66	Total	O	0	0
			66	66		
4	C	70	Total	O	0	0
			70	70		
4	D	59	Total	O	0	0
			59	59		

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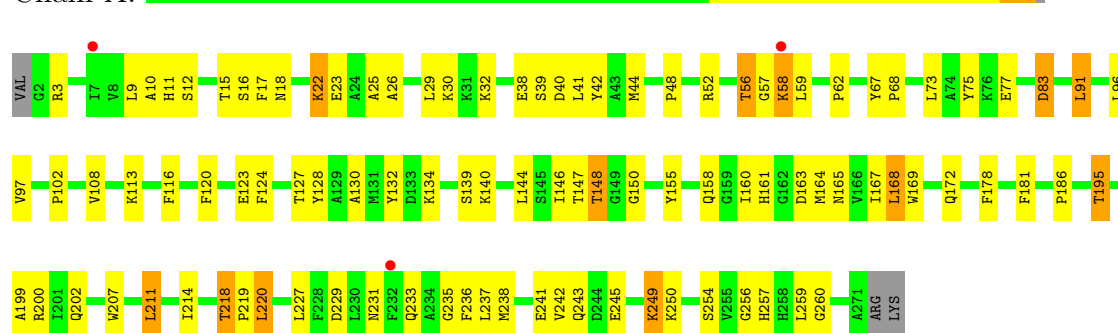
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	37	Total 37	O 37	0	0
4	F	41	Total 41	O 41	0	0
4	G	54	Total 54	O 54	0	0
4	H	41	Total 41	O 41	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

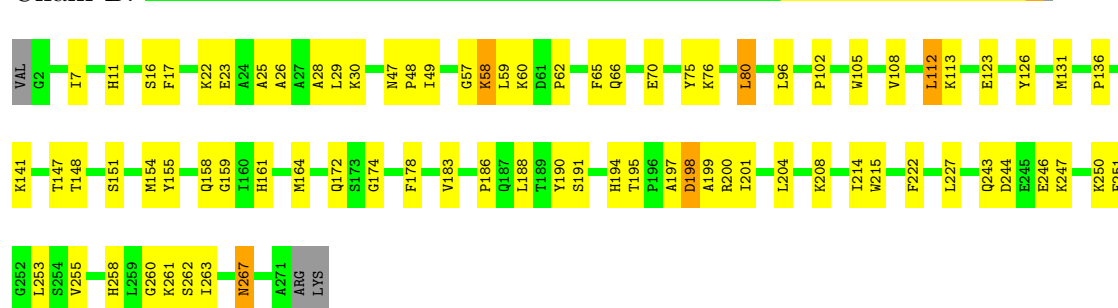
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain A:



- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain B:



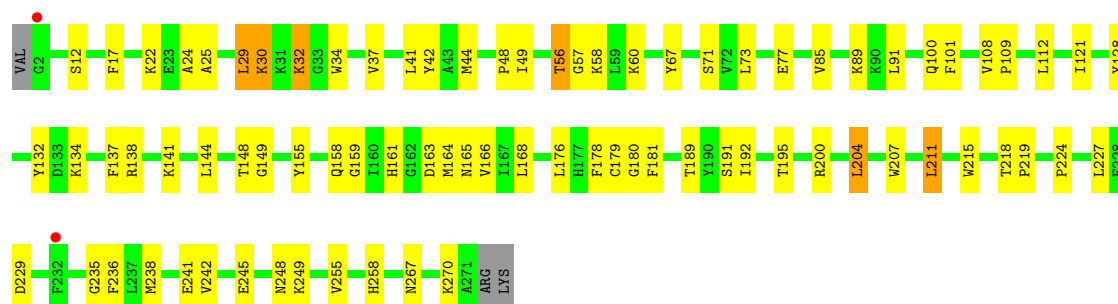
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain C:



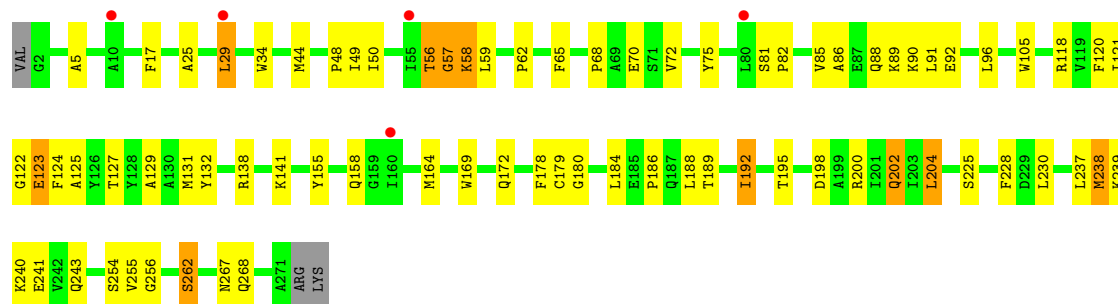
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain D:



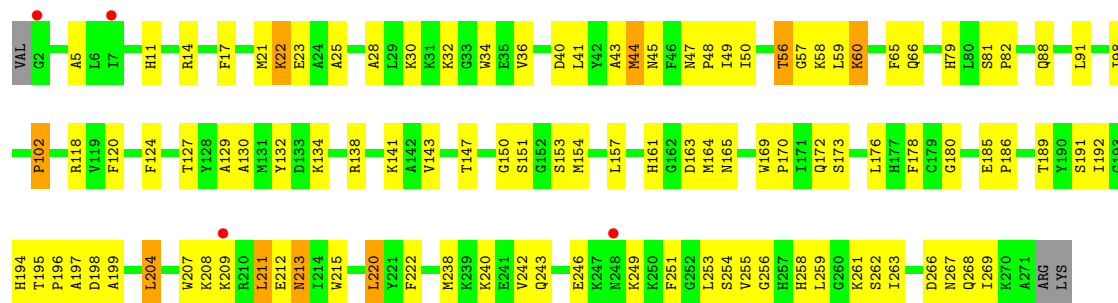
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain E:



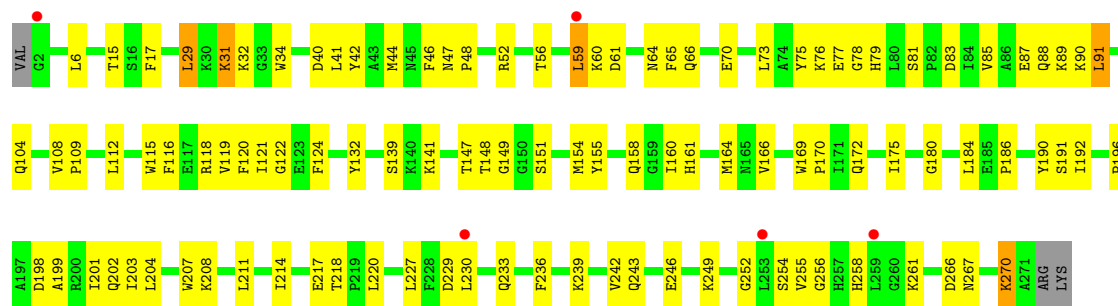
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain F:



- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

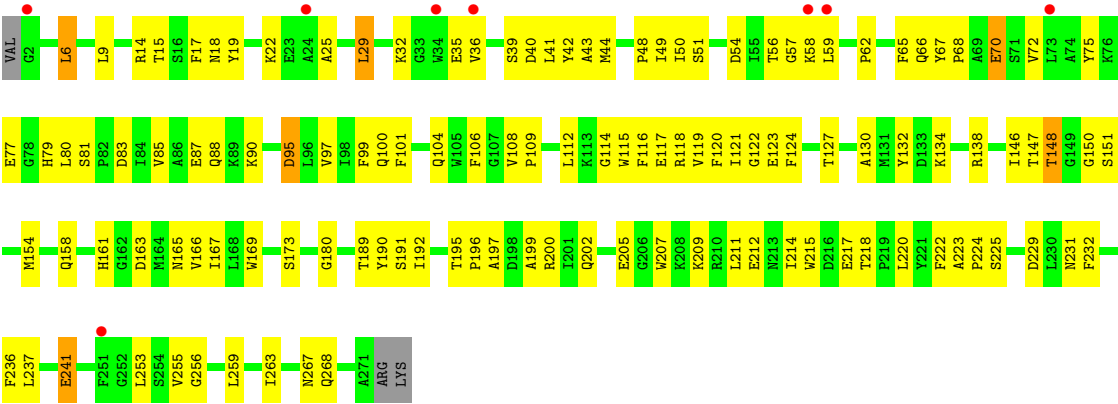
Chain G:



- Molecule 1: NAD(P)H dehydrogenase [quinone] 1



Chain H: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.04Å 209.94Å 102.08Å 90.00° 109.93° 90.00°	Depositor
Resolution (Å)	47.95 – 2.45 47.95 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.95-2.45) 99.1 (47.95-2.45)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.206 , 0.269 0.206 , 0.270	Depositor DCC
$R_{free}$ test set	5062 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.9	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.6	EDS
Estimated twinning fraction	0.199 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 101125 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18234	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.51% 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: FAD, CC2

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	0/2205	0.59	0/2980
1	B	0.46	0/2205	0.58	0/2980
1	C	0.45	0/2205	0.58	0/2980
1	D	0.46	0/2205	0.58	0/2980
1	E	0.40	0/2205	0.54	0/2980
1	F	0.41	0/2205	0.57	0/2980
1	G	0.41	0/2205	0.56	0/2980
1	H	0.40	0/2205	0.55	0/2980
All	All	0.43	0/17640	0.57	0/23840

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2147	0	2141	90	0
1	B	2147	0	2141	79	0
1	C	2147	0	2141	80	0
1	D	2147	0	2141	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2147	0	2141	70	0
1	F	2147	0	2141	89	0
1	G	2147	0	2141	75	0
1	H	2147	0	2141	99	0
2	A	53	0	31	7	0
2	B	53	0	31	10	0
2	C	53	0	31	6	0
2	D	53	0	31	6	0
2	E	53	0	31	4	0
2	F	53	0	31	4	0
2	G	53	0	31	2	0
2	H	53	0	31	9	0
3	A	25	0	17	1	0
3	B	25	0	18	10	0
3	C	25	0	17	4	0
3	D	25	0	17	2	0
3	E	25	0	18	3	0
3	F	25	0	18	3	0
3	G	25	0	18	2	0
3	H	25	0	17	3	0
4	A	66	0	0	2	0
4	B	66	0	0	0	0
4	C	70	0	0	2	0
4	D	59	0	0	4	0
4	E	37	0	0	4	0
4	F	41	0	0	2	0
4	G	54	0	0	2	0
4	H	41	0	0	2	0
All	All	18234	0	17516	626	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 18.

All (626) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:228:PHE:HA	4:E:361:HOH:O	1.37	1.22
1:F:151:SER:H	1:F:154:MET:HE3	1.08	1.12
1:F:17:PHE:HB2	2:F:601:FAD:H52A	1.13	1.11
1:B:17:PHE:HB2	2:B:601:FAD:H52A	1.13	1.07
1:E:238:MET:HA	4:E:361:HOH:O	1.54	1.05
1:C:14:ARG:HH11	1:C:14:ARG:HG3	1.25	1.02
1:A:158:GLN:HG2	1:B:243:GLN:HE21	1.26	1.01

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:172:GLN:HG2	1:B:183:VAL:HG11	1.43	1.00
1:B:194:HIS:CE1	3:B:547:CC2:H21	1.98	0.97
1:E:141:LYS:HD3	1:E:184:LEU:HD11	1.48	0.93
1:H:50:ILE:HD12	1:H:117:GLU:HB3	1.50	0.92
1:C:243:GLN:HE21	1:D:158:GLN:HG2	1.36	0.90
1:G:148:THR:HG22	1:G:190:TYR:HA	1.54	0.90
1:H:130:ALA:HB1	1:H:134:LYS:HB2	1.54	0.89
1:B:147:THR:OG1	2:B:601:FAD:H5'2	1.73	0.88
1:F:17:PHE:CB	2:F:601:FAD:H52A	2.01	0.88
1:A:158:GLN:HG2	1:B:243:GLN:NE2	1.90	0.86
1:E:172:GLN:HE22	1:E:186:PRO:HG3	1.42	0.83
1:B:17:PHE:HB2	2:B:601:FAD:C5B	2.06	0.83
1:B:148:THR:HG22	1:B:190:TYR:HA	1.60	0.83
1:G:47:ASN:HB3	1:G:118:ARG:NH1	1.94	0.83
1:F:151:SER:H	1:F:154:MET:CE	1.92	0.82
1:C:17:PHE:HB2	2:C:601:FAD:H52A	1.61	0.81
1:A:9:LEU:HD22	1:A:22:LYS:HG2	1.62	0.81
1:H:127:THR:HG22	1:H:130:ALA:H	1.45	0.81
1:A:164:MET:HE3	1:A:167:ILE:HB	1.63	0.80
1:H:65:PHE:CE1	1:H:70:GLU:HG2	2.17	0.80
1:F:151:SER:N	1:F:154:MET:HE3	1.93	0.80
1:C:224:PRO:HD2	1:C:227:LEU:HD22	1.63	0.80
1:A:113:LYS:NZ	1:B:105:TRP:HB2	1.97	0.79
1:A:147:THR:OG1	2:A:601:FAD:H5'2	1.83	0.79
1:E:169:TRP:CZ2	1:E:256:GLY:HA3	2.19	0.78
1:G:65:PHE:CE1	1:G:70:GLU:HG2	2.17	0.78
1:E:56:THR:HG22	1:E:57:GLY:H	1.48	0.78
1:A:163:ASP:OD2	1:A:165:ASN:HB2	1.83	0.78
1:E:267:ASN:ND2	1:E:268:GLN:HE21	1.83	0.77
1:G:65:PHE:HE1	1:G:70:GLU:HG2	1.46	0.77
1:B:7:ILE:HG21	1:B:22:LYS:HG2	1.65	0.77
1:C:243:GLN:NE2	1:D:158:GLN:HG2	2.01	0.76
1:G:198:ASP:HA	1:G:201:ILE:HD13	1.67	0.76
1:F:132:TYR:OH	1:H:161:HIS:HD2	1.68	0.75
1:C:48:PRO:HG3	1:D:49:ILE:HD11	1.68	0.75
1:E:17:PHE:HB2	2:E:601:FAD:H52A	1.67	0.75
1:B:147:THR:HG1	2:B:601:FAD:H5'2	1.48	0.75
1:H:147:THR:OG1	2:H:601:FAD:H5'2	1.86	0.74
1:F:60:LYS:HD3	1:F:60:LYS:O	1.88	0.74
1:C:255:VAL:HG23	1:C:267:ASN:HD22	1.53	0.74
1:E:58:LYS:HD3	1:E:58:LYS:N	2.02	0.74
1:E:58:LYS:H	1:E:58:LYS:HD3	1.52	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:58:LYS:HD3	1:C:58:LYS:H	1.54	0.73
1:A:164:MET:HE2	1:A:168:LEU:HD13	1.69	0.73
1:C:172:GLN:HG2	1:C:183:VAL:HG11	1.70	0.73
1:A:17:PHE:HB2	2:A:601:FAD:H51A	1.71	0.72
1:G:56:THR:HG23	1:G:79:HIS:O	1.88	0.72
1:B:17:PHE:CB	2:B:601:FAD:H52A	2.07	0.72
1:G:246:GLU:OE1	1:G:249:LYS:HD2	1.90	0.72
1:B:161:HIS:HE1	3:B:547:CC2:O7	1.73	0.72
1:F:153:SER:OG	1:H:237:LEU:HD21	1.90	0.71
1:D:85:VAL:O	1:D:89:LYS:HG2	1.90	0.71
1:E:132:TYR:OH	1:G:161:HIS:HD2	1.72	0.71
1:A:164:MET:CE	1:A:168:LEU:HD13	2.20	0.71
1:C:164:MET:SD	1:C:168:LEU:HD13	2.31	0.71
1:A:128:TYR:HE1	3:B:547:CC2:HO1	1.38	0.69
1:F:169:TRP:CZ2	1:F:256:GLY:HA3	2.27	0.69
1:H:138:ARG:HA	1:H:180:GLY:O	1.92	0.69
1:A:9:LEU:HD12	1:A:10:ALA:H	1.58	0.69
1:B:255:VAL:HG23	1:B:267:ASN:HD22	1.58	0.68
1:E:75:TYR:CZ	1:E:124:PHE:HB2	2.28	0.68
1:F:25:ALA:HB2	1:F:207:TRP:HE1	1.59	0.68
1:G:255:VAL:HG23	1:G:267:ASN:HD22	1.58	0.68
1:C:17:PHE:HB2	2:C:601:FAD:C5B	2.24	0.68
1:A:257:HIS:HD2	4:A:326:HOH:O	1.77	0.67
1:C:144:LEU:HD22	1:C:172:GLN:HE21	1.59	0.67
1:F:204:LEU:O	1:F:208:LYS:HG3	1.93	0.67
1:H:173:SER:HB2	1:H:222:PHE:CE1	2.28	0.67
1:H:108:VAL:HG13	1:H:112:LEU:HB3	1.76	0.67
1:B:148:THR:CG2	1:B:190:TYR:HA	2.25	0.67
1:C:14:ARG:HH11	1:C:14:ARG:CG	2.06	0.66
1:E:255:VAL:HG23	1:E:267:ASN:HD22	1.60	0.66
1:H:81:SER:O	1:H:85:VAL:HG23	1.96	0.66
1:G:31:LYS:HG3	1:G:32:LYS:N	2.10	0.66
1:C:176:LEU:O	1:C:181:PHE:HB2	1.95	0.66
1:C:50:ILE:HG22	1:C:118:ARG:HG2	1.77	0.66
1:G:41:LEU:HA	1:G:44:MET:HE2	1.78	0.66
1:D:17:PHE:HB2	2:D:601:FAD:H52A	1.78	0.66
1:H:17:PHE:HB2	2:H:601:FAD:H52A	1.78	0.65
1:H:255:VAL:HG23	1:H:267:ASN:HD22	1.62	0.65
1:A:148:THR:CG2	1:A:150:GLY:O	2.44	0.65
1:D:56:THR:HG22	1:D:57:GLY:N	2.12	0.65
1:F:141:LYS:HD2	1:F:215:TRP:CE3	2.31	0.65
1:B:25:ALA:O	1:B:29:LEU:HB2	1.97	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:172:GLN:HE22	1:F:186:PRO:HG3	1.62	0.65
1:E:17:PHE:HB2	2:E:601:FAD:C5B	2.25	0.65
1:H:173:SER:HB2	1:H:222:PHE:HE1	1.62	0.65
1:H:14:ARG:HA	1:H:19:TYR:CD1	2.31	0.64
1:A:200:ARG:NH1	2:A:601:FAD:N3A	2.45	0.64
1:F:138:ARG:HA	1:F:180:GLY:O	1.97	0.64
1:E:237:LEU:O	4:E:361:HOH:O	2.14	0.64
1:F:258:HIS:CE1	1:H:263:ILE:HD12	2.32	0.64
1:H:88:GLN:HG2	1:H:124:PHE:CE2	2.32	0.64
2:B:601:FAD:H9	2:B:601:FAD:O2'	1.97	0.64
1:F:246:GLU:HA	1:F:249:LYS:HG3	1.79	0.64
1:B:255:VAL:HA	1:B:263:ILE:HD13	1.79	0.64
1:A:48:PRO:HG3	1:B:49:ILE:HD11	1.80	0.64
1:H:18:ASN:ND2	1:H:100:GLN:HE21	1.96	0.63
1:B:250:LYS:HE2	1:B:251:PHE:CE2	2.34	0.63
1:D:17:PHE:HB2	2:D:601:FAD:C5B	2.29	0.63
1:H:148:THR:HG22	1:H:190:TYR:HA	1.81	0.62
1:D:67:TYR:O	1:D:71:SER:HB3	1.99	0.62
1:B:108:VAL:HG13	1:B:112:LEU:HB3	1.80	0.62
1:E:56:THR:HG22	1:E:57:GLY:N	2.14	0.61
1:G:116:PHE:O	1:G:120:PHE:HB2	2.00	0.61
1:F:25:ALA:HA	1:F:211:LEU:HD23	1.83	0.61
1:F:91:LEU:HD21	1:F:120:PHE:HE1	1.65	0.61
1:B:198:ASP:HA	1:B:201:ILE:HD13	1.82	0.61
1:B:151:SER:OG	1:B:154:MET:HG3	2.00	0.61
1:A:260:GLY:O	1:B:262:SER:OG	2.16	0.61
1:H:50:ILE:HG12	1:H:67:TYR:CZ	2.36	0.61
1:H:17:PHE:HB2	2:H:601:FAD:C5B	2.31	0.61
1:D:73:LEU:HD11	1:D:77:GLU:OE2	2.00	0.61
1:B:59:LEU:HB2	1:B:62:PRO:HG3	1.83	0.61
1:A:3:ARG:HH11	1:A:3:ARG:HG2	1.66	0.61
1:F:189:THR:CG2	1:F:192:ILE:HD13	2.30	0.60
1:F:154:MET:O	1:F:161:HIS:HB2	2.01	0.60
1:H:40:ASP:HB3	1:H:43:ALA:HB3	1.84	0.60
1:A:113:LYS:HZ1	1:B:105:TRP:HB2	1.65	0.60
1:C:108:VAL:HG22	1:C:112:LEU:HD23	1.83	0.60
1:F:60:LYS:HD3	1:F:60:LYS:C	2.21	0.60
1:C:58:LYS:N	1:C:58:LYS:HD3	2.15	0.60
1:A:75:TYR:CZ	1:A:124:PHE:HB2	2.37	0.60
1:H:77:GLU:HB3	1:H:79:HIS:CD2	2.37	0.59
1:H:229:ASP:O	1:H:236:PHE:HA	2.03	0.59
1:A:16:SER:HA	2:A:601:FAD:O1A	2.02	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:207:TRP:O	1:H:211:LEU:HG	2.01	0.59
1:A:200:ARG:NH1	2:A:601:FAD:H1B	2.17	0.59
1:E:49:ILE:HD11	1:G:48:PRO:HG2	1.83	0.59
1:A:128:TYR:HD1	3:B:547:CC2:C18	2.16	0.59
1:G:77:GLU:O	1:G:79:HIS:HD2	1.85	0.59
1:H:220:LEU:HD21	1:H:268:GLN:O	2.02	0.59
1:D:41:LEU:HA	1:D:44:MET:HE3	1.85	0.59
1:H:39:SER:HA	1:H:44:MET:HE1	1.84	0.59
1:C:25:ALA:HA	1:C:211:LEU:HD23	1.84	0.59
2:E:601:FAD:H9	2:E:601:FAD:O2'	2.03	0.58
1:H:75:TYR:CZ	1:H:124:PHE:HB2	2.38	0.58
1:G:52:ARG:HB3	1:G:59:LEU:HD21	1.84	0.58
1:A:41:LEU:HA	1:A:44:MET:HE3	1.85	0.58
1:C:147:THR:OG1	2:C:601:FAD:H5'2	2.04	0.58
1:E:241:GLU:CD	1:E:241:GLU:H	2.04	0.58
1:G:17:PHE:HB2	2:G:601:FAD:H51A	1.85	0.58
1:A:144:LEU:HD23	1:A:146:ILE:HD11	1.85	0.58
1:C:122:GLY:O	1:C:124:PHE:N	2.34	0.58
1:C:50:ILE:CG2	1:C:118:ARG:HG2	2.34	0.58
1:F:243:GLN:NE2	1:H:158:GLN:HG2	2.19	0.58
1:E:239:LYS:O	1:E:243:GLN:HG3	2.03	0.58
1:H:50:ILE:HG13	1:H:118:ARG:HG2	1.84	0.58
1:A:249:LYS:HD3	1:A:250:LYS:N	2.18	0.57
1:C:198:ASP:O	1:C:202:GLN:HG2	2.04	0.57
1:A:128:TYR:HE1	3:B:547:CC2:O1	1.86	0.57
1:C:238:MET:CE	1:C:242:VAL:HG12	2.34	0.57
1:H:32:LYS:HG3	1:H:212:GLU:HA	1.85	0.57
1:A:56:THR:HG22	1:A:57:GLY:N	2.17	0.57
1:G:47:ASN:HB3	1:G:118:ARG:HH12	1.69	0.57
1:G:81:SER:O	1:G:85:VAL:HG23	2.04	0.57
1:G:42:TYR:HB2	4:G:281:HOH:O	2.04	0.57
1:C:21:MET:HG3	1:C:207:TRP:CD1	2.39	0.57
1:F:25:ALA:HB2	1:F:207:TRP:NE1	2.19	0.57
1:H:54:ASP:OD1	4:H:290:HOH:O	2.18	0.57
1:C:17:PHE:CZ	1:C:204:LEU:HD13	2.40	0.57
2:D:601:FAD:O4'	2:D:601:FAD:O2'	2.13	0.57
1:A:22:LYS:HE3	1:A:23:GLU:OE1	2.05	0.57
1:B:141:LYS:HE3	1:B:215:TRP:CE2	2.40	0.57
1:A:25:ALA:HB2	1:A:207:TRP:HE1	1.70	0.56
1:G:148:THR:CG2	1:G:190:TYR:HA	2.33	0.56
1:H:39:SER:HA	1:H:44:MET:CE	2.35	0.56
1:A:75:TYR:CE1	1:A:124:PHE:HB2	2.41	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:48:PRO:HG2	1:E:49:ILE:HD12	1.88	0.56
1:H:116:PHE:O	1:H:120:PHE:HB2	2.05	0.56
2:D:601:FAD:HO4'	2:D:601:FAD:HO2'	1.47	0.56
1:F:164:MET:O	1:F:164:MET:HG3	2.05	0.56
1:A:231:ASN:OD1	1:A:233:GLN:HB2	2.06	0.56
1:G:66:GLN:O	1:G:70:GLU:HB2	2.05	0.56
1:D:138:ARG:HA	1:D:180:GLY:O	2.05	0.56
1:E:138:ARG:HA	1:E:180:GLY:O	2.05	0.56
1:G:147:THR:OG1	2:G:601:FAD:H5'2	2.05	0.56
1:D:108:VAL:HG13	1:D:112:LEU:HB3	1.87	0.56
1:B:197:ALA:O	1:B:201:ILE:CD1	2.53	0.56
1:H:253:LEU:N	1:H:253:LEU:HD12	2.21	0.56
1:D:161:HIS:HE1	3:D:547:CC2:O7	1.89	0.56
1:G:214:ILE:HD12	1:G:217:GLU:OE1	2.06	0.55
1:C:186:PRO:HD2	4:C:300:HOH:O	2.06	0.55
3:E:547:CC2:O7	3:E:547:CC2:H19	2.05	0.55
1:F:141:LYS:HD2	1:F:215:TRP:CZ3	2.41	0.55
1:G:184:LEU:HD12	1:G:184:LEU:N	2.22	0.55
1:E:131:MET:HE2	1:E:178:PHE:HE1	1.72	0.55
1:E:225:SER:HB2	1:E:230:LEU:HD21	1.89	0.55
1:A:202:GLN:HB3	1:H:202:GLN:HB3	1.89	0.55
1:A:172:GLN:HE22	1:A:186:PRO:HD3	1.72	0.55
1:C:9:LEU:HD22	1:C:22:LYS:HD2	1.88	0.55
1:C:155:TYR:HB3	1:C:164:MET:HB2	1.89	0.54
1:F:173:SER:HB2	1:F:222:PHE:CE1	2.42	0.54
1:G:242:VAL:O	1:G:246:GLU:HG2	2.07	0.54
1:B:201:ILE:H	1:B:201:ILE:HD12	1.73	0.54
1:F:48:PRO:HG3	1:H:49:ILE:HD11	1.90	0.54
1:A:241:GLU:O	1:A:245:GLU:HG3	2.07	0.54
1:A:148:THR:HG21	1:A:150:GLY:O	2.07	0.54
1:A:140:LYS:HB2	1:A:181:PHE:CE1	2.42	0.54
1:D:195:THR:O	1:D:200:ARG:HD3	2.07	0.54
1:D:248:ASN:HB2	4:D:339:HOH:O	2.08	0.54
1:H:81:SER:HB3	1:H:83:ASP:OD1	2.08	0.54
1:A:195:THR:HG22	1:A:199:ALA:HB3	1.90	0.54
1:E:237:LEU:HD22	1:G:158:GLN:HB2	1.90	0.54
1:A:113:LYS:HZ2	1:B:105:TRP:HB2	1.69	0.54
1:H:215:TRP:O	1:H:215:TRP:CD1	2.61	0.54
1:G:252:GLY:HA3	1:G:258:HIS:HA	1.90	0.54
1:A:229:ASP:O	1:A:236:PHE:HA	2.08	0.54
1:F:249:LYS:NZ	4:F:280:HOH:O	2.41	0.53
1:F:91:LEU:HD21	1:F:120:PHE:CE1	2.43	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:161:HIS:HD2	1:D:132:TYR:OH	1.90	0.53
1:B:11:HIS:NE2	2:B:601:FAD:O2P	2.41	0.53
1:C:164:MET:SD	1:C:167:ILE:HD12	2.49	0.53
1:C:14:ARG:HG3	1:C:14:ARG:NH1	2.03	0.53
1:E:155:TYR:HB3	1:E:164:MET:HB2	1.90	0.53
1:A:160:ILE:O	1:A:160:ILE:HG13	2.07	0.53
1:A:59:LEU:HB2	1:A:62:PRO:HG3	1.90	0.53
2:H:601:FAD:H9	2:H:601:FAD:O2'	2.09	0.53
1:B:201:ILE:HD12	1:B:201:ILE:N	2.23	0.53
1:B:197:ALA:HA	1:B:200:ARG:CZ	2.38	0.53
1:D:12:SER:HB3	1:D:42:TYR:CE1	2.44	0.53
1:D:148:THR:HG23	2:D:601:FAD:O2	2.09	0.53
1:F:59:LEU:HD13	1:F:65:PHE:CD1	2.44	0.53
1:E:238:MET:CA	4:E:361:HOH:O	2.31	0.52
1:B:75:TYR:HA	1:B:80:LEU:HD22	1.90	0.52
1:B:194:HIS:CE1	3:B:547:CC2:C21	2.82	0.52
1:F:132:TYR:CD1	1:F:178:PHE:HA	2.44	0.52
1:G:172:GLN:HE22	1:G:186:PRO:HG3	1.73	0.52
1:G:83:ASP:O	1:G:87:GLU:HG2	2.08	0.52
1:B:58:LYS:H	1:B:58:LYS:HD2	1.74	0.52
1:H:68:PRO:O	1:H:72:VAL:HG23	2.08	0.52
1:G:31:LYS:HG3	1:G:32:LYS:H	1.73	0.52
1:H:169:TRP:CZ2	1:H:256:GLY:HA3	2.44	0.52
1:A:26:ALA:O	1:A:30:LYS:HG3	2.09	0.52
1:G:196:PRO:O	1:G:199:ALA:HB3	2.10	0.52
1:B:65:PHE:CE1	1:B:70:GLU:HG2	2.45	0.52
1:G:161:HIS:HE1	3:G:547:CC2:O7	1.92	0.52
1:A:39:SER:HB3	1:A:44:MET:HE1	1.92	0.52
1:F:40:ASP:O	1:F:44:MET:HG3	2.09	0.52
1:F:169:TRP:HB3	1:F:170:PRO:HD3	1.92	0.52
1:G:75:TYR:CZ	1:G:124:PHE:HB2	2.45	0.52
1:C:196:PRO:O	1:C:199:ALA:HB3	2.10	0.52
1:B:131:MET:HE2	1:B:178:PHE:HE1	1.75	0.52
1:G:151:SER:OG	1:G:154:MET:HG3	2.10	0.52
1:B:197:ALA:O	1:B:201:ILE:HD12	2.09	0.51
1:D:60:LYS:HD3	1:D:73:LEU:CD2	2.40	0.51
1:H:83:ASP:O	1:H:87:GLU:HG2	2.10	0.51
1:A:41:LEU:HD23	1:A:44:MET:CE	2.40	0.51
1:F:147:THR:OG1	2:F:601:FAD:H5'2	2.11	0.51
1:H:77:GLU:HB3	1:H:79:HIS:NE2	2.25	0.51
1:G:199:ALA:O	1:G:203:ILE:HG13	2.10	0.51
1:B:148:THR:HG23	1:B:191:SER:H	1.75	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:164:MET:SD	1:C:167:ILE:CD1	2.98	0.51
1:E:198:ASP:O	1:E:202:GLN:HG2	2.11	0.51
1:E:59:LEU:HD13	1:E:65:PHE:CD1	2.45	0.51
1:A:40:ASP:N	1:A:44:MET:HE2	2.26	0.51
1:C:238:MET:HE2	1:C:242:VAL:HG12	1.93	0.51
1:D:141:LYS:HG3	1:D:215:TRP:CZ3	2.45	0.51
1:G:141:LYS:HB3	1:G:184:LEU:HD11	1.93	0.51
1:G:169:TRP:CZ2	1:G:256:GLY:HA3	2.45	0.51
1:D:238:MET:HE2	1:D:242:VAL:HG12	1.91	0.51
1:H:65:PHE:HE1	1:H:70:GLU:HG2	1.72	0.51
1:D:229:ASP:O	1:D:236:PHE:HA	2.11	0.51
1:E:89:LYS:O	1:E:92:GLU:HB2	2.10	0.51
1:H:66:GLN:HG3	1:H:68:PRO:HD2	1.92	0.50
1:F:32:LYS:HE3	1:F:212:GLU:HB3	1.93	0.50
1:B:26:ALA:O	1:B:30:LYS:HG3	2.10	0.50
1:D:176:LEU:O	1:D:181:PHE:HB2	2.11	0.50
1:F:50:ILE:CG2	1:F:118:ARG:HG2	2.41	0.50
1:F:50:ILE:HG22	1:F:118:ARG:HG2	1.94	0.50
1:A:211:LEU:O	1:A:214:ILE:HG22	2.11	0.50
1:E:81:SER:O	1:E:85:VAL:HG23	2.11	0.50
1:G:204:LEU:O	1:G:208:LYS:HG2	2.12	0.50
1:F:169:TRP:CD1	1:H:166:VAL:HG11	2.46	0.50
1:H:108:VAL:HG12	1:H:109:PRO:O	2.11	0.50
1:F:246:GLU:CD	1:F:253:LEU:HD11	2.32	0.50
1:D:25:ALA:O	1:D:29:LEU:HD23	2.11	0.50
1:F:259:LEU:HB2	1:F:261:LYS:HE2	1.93	0.50
1:H:95:ASP:HB3	1:H:215:TRP:CZ3	2.47	0.50
1:E:195:THR:O	1:E:200:ARG:HD3	2.11	0.50
1:A:161:HIS:HE1	3:A:547:CC2:O7	1.95	0.50
1:H:9:LEU:HD22	1:H:22:LYS:HD3	1.92	0.49
2:E:601:FAD:H3B	2:E:601:FAD:O1A	2.12	0.49
1:H:253:LEU:H	1:H:253:LEU:HD12	1.77	0.49
1:F:251:PHE:CD1	1:F:262:SER:HB2	2.47	0.49
1:A:148:THR:HG22	1:A:150:GLY:O	2.10	0.49
1:D:144:LEU:HD21	1:D:176:LEU:HD11	1.94	0.49
1:D:137:PHE:CD2	1:D:179:CYS:HB3	2.47	0.49
1:A:254:SER:HB2	1:A:257:HIS:HB2	1.94	0.49
1:A:164:MET:HE3	1:A:167:ILE:CB	2.38	0.49
1:G:40:ASP:O	1:G:44:MET:HG3	2.12	0.49
1:E:49:ILE:HD11	1:G:48:PRO:CG	2.42	0.49
3:B:547:CC2:C8	3:B:547:CC2:H19	2.42	0.49
1:A:257:HIS:HE1	1:B:159:GLY:O	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:195:THR:HG22	1:B:199:ALA:HB3	1.94	0.49
1:E:29:LEU:HD12	1:E:34:TRP:CD1	2.48	0.49
1:A:39:SER:C	1:A:44:MET:HE2	2.33	0.49
1:B:131:MET:HE2	1:B:178:PHE:CE1	2.48	0.49
1:H:95:ASP:HB3	1:H:215:TRP:CH2	2.48	0.49
1:E:48:PRO:HG2	1:E:49:ILE:CD1	2.43	0.49
1:C:29:LEU:O	1:C:34:TRP:HB2	2.13	0.49
1:H:127:THR:HG22	1:H:130:ALA:N	2.21	0.48
2:H:601:FAD:C4	3:H:547:CC2:C2	2.91	0.48
1:D:29:LEU:HD21	1:D:211:LEU:HG	1.95	0.48
1:A:67:TYR:N	1:A:68:PRO:CD	2.76	0.48
1:H:134:LYS:HE2	1:H:225:SER:OG	2.14	0.48
1:C:167:ILE:C	1:C:167:ILE:HD13	2.33	0.48
1:H:151:SER:OG	1:H:154:MET:HG3	2.14	0.48
1:F:255:VAL:HG22	1:F:263:ILE:HG21	1.95	0.48
1:C:122:GLY:C	1:C:124:PHE:H	2.15	0.48
1:C:122:GLY:HA2	1:C:126:TYR:CE2	2.48	0.48
1:F:173:SER:HB2	1:F:222:PHE:HE1	1.78	0.48
1:D:238:MET:CE	1:D:242:VAL:HG12	2.43	0.48
1:C:91:LEU:HD21	1:C:115:TRP:CH2	2.49	0.48
3:C:547:CC2:H19	3:C:547:CC2:C8	2.43	0.48
1:C:60:LYS:O	1:C:60:LYS:HG3	2.14	0.48
1:H:122:GLY:O	1:H:123:GLU:HB3	2.13	0.48
1:F:189:THR:HG21	1:F:192:ILE:HD13	1.95	0.48
1:C:241:GLU:HG2	1:C:242:VAL:H	1.78	0.48
1:B:246:GLU:O	1:B:261:LYS:NZ	2.46	0.48
1:D:158:GLN:NE2	4:D:344:HOH:O	2.47	0.48
1:A:3:ARG:NH1	1:A:3:ARG:HG2	2.29	0.48
1:A:249:LYS:HD3	1:A:250:LYS:H	1.78	0.48
1:B:76:LYS:HE3	1:B:123:GLU:OE1	2.14	0.47
1:G:184:LEU:CD1	1:G:184:LEU:N	2.76	0.47
1:E:59:LEU:HD13	1:E:65:PHE:HD1	1.80	0.47
1:F:56:THR:CG2	1:F:57:GLY:N	2.77	0.47
1:C:138:ARG:HA	1:C:180:GLY:O	2.14	0.47
1:B:23:GLU:HA	1:B:23:GLU:OE1	2.14	0.47
1:C:263:ILE:HD12	1:D:258:HIS:CE1	2.50	0.47
1:A:238:MET:HE3	1:A:243:GLN:HG2	1.95	0.47
1:E:131:MET:CE	1:E:178:PHE:HE1	2.26	0.47
1:A:169:TRP:CZ2	1:A:256:GLY:HA3	2.49	0.47
1:D:71:SER:OG	1:D:121:ILE:HD12	2.14	0.47
1:F:194:HIS:CE1	1:H:232:PHE:CZ	3.02	0.47
1:H:197:ALA:HA	1:H:200:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:194:HIS:HE1	3:B:547:CC2:H21	1.67	0.47
1:C:147:THR:HG1	2:C:601:FAD:H5'2	1.79	0.47
1:A:200:ARG:NH1	2:A:601:FAD:C1B	2.78	0.47
1:C:164:MET:SD	1:C:168:LEU:CD1	3.03	0.47
1:C:214:ILE:O	1:C:217:GLU:HG3	2.14	0.47
1:D:255:VAL:HG23	1:D:267:ASN:HD22	1.79	0.47
1:H:214:ILE:HG23	1:H:215:TRP:N	2.29	0.47
1:F:40:ASP:HB3	1:F:43:ALA:HB3	1.97	0.47
1:H:56:THR:HG22	1:H:57:GLY:N	2.29	0.47
1:C:14:ARG:NH1	1:C:14:ARG:CG	2.69	0.47
1:E:132:TYR:OH	1:G:161:HIS:CD2	2.60	0.47
1:F:185:GLU:HG2	1:F:269:ILE:O	2.15	0.47
1:B:141:LYS:HE3	1:B:215:TRP:CZ2	2.50	0.47
1:E:91:LEU:HD21	1:E:120:PHE:CE1	2.50	0.47
1:A:132:TYR:OH	1:B:161:HIS:HD2	1.98	0.47
1:C:141:LYS:HD2	1:C:215:TRP:CE3	2.50	0.47
1:E:120:PHE:HA	1:E:125:ALA:HB2	1.97	0.47
1:C:153:SER:OG	1:D:235:GLY:O	2.33	0.47
1:D:60:LYS:HD3	1:D:73:LEU:HD21	1.96	0.46
1:E:59:LEU:HB2	1:E:62:PRO:HG3	1.97	0.46
1:B:258:HIS:CD2	1:B:260:GLY:H	2.33	0.46
3:C:547:CC2:H19	3:C:547:CC2:O7	2.15	0.46
1:G:121:ILE:HG22	1:G:122:GLY:N	2.31	0.46
1:H:189:THR:CG2	1:H:192:ILE:HD13	2.45	0.46
1:G:61:ASP:OD2	1:G:64:ASN:HB3	2.15	0.46
1:A:128:TYR:HD1	3:B:547:CC2:C19	2.28	0.46
1:F:22:LYS:HD2	1:F:22:LYS:C	2.35	0.46
1:D:24:ALA:HB2	1:D:204:LEU:HD12	1.97	0.46
1:D:155:TYR:HB3	1:D:164:MET:HB2	1.96	0.46
1:A:73:LEU:HD11	1:A:77:GLU:OE2	2.15	0.46
1:H:6:LEU:HD13	1:H:90:LYS:HB3	1.95	0.46
1:F:169:TRP:CD1	1:H:166:VAL:CG1	2.98	0.46
1:E:86:ALA:O	1:E:90:LYS:HG3	2.15	0.46
1:G:266:ASP:HB3	1:G:270:LYS:HB2	1.97	0.46
1:C:30:LYS:HE3	1:C:36:VAL:HB	1.97	0.46
1:G:91:LEU:HD21	1:G:120:PHE:HE1	1.81	0.46
1:G:172:GLN:NE2	4:G:291:HOH:O	2.48	0.46
3:G:547:CC2:C8	3:G:547:CC2:H19	2.45	0.46
1:F:212:GLU:HB2	1:F:213:ASN:ND2	2.30	0.46
1:G:202:GLN:HA	1:G:202:GLN:NE2	2.30	0.46
1:D:137:PHE:HB2	1:D:179:CYS:O	2.16	0.46
1:C:73:LEU:HD11	1:C:77:GLU:CD	2.36	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:106:PHE:HD1	1:H:167:ILE:HD13	1.80	0.46
4:A:311:HOH:O	1:B:222:PHE:HB3	2.15	0.46
1:H:148:THR:HG23	1:H:150:GLY:O	2.16	0.45
1:D:30:LYS:HE3	1:D:30:LYS:HB3	1.50	0.45
1:C:111:ILE:HD12	1:D:49:ILE:HD13	1.99	0.45
1:B:59:LEU:HD12	1:B:62:PRO:HB3	1.97	0.45
1:A:32:LYS:HD3	1:A:32:LYS:HA	1.78	0.45
1:E:81:SER:HA	1:E:82:PRO:HD3	1.86	0.45
1:F:88:GLN:HG2	1:F:124:PHE:CE2	2.52	0.45
1:G:115:TRP:O	1:G:119:VAL:HB	2.17	0.45
1:F:163:ASP:OD2	1:F:165:ASN:HB2	2.16	0.45
1:G:31:LYS:CG	1:G:32:LYS:N	2.78	0.45
1:F:48:PRO:HD2	1:F:49:ILE:HG13	1.98	0.45
1:G:169:TRP:HB3	1:G:170:PRO:HD3	1.99	0.45
1:A:130:ALA:HB1	1:A:134:LYS:O	2.16	0.45
1:A:96:LEU:HD12	1:A:97:VAL:N	2.32	0.45
1:C:67:TYR:N	1:C:68:PRO:CD	2.79	0.45
1:D:108:VAL:HG13	1:D:112:LEU:HD23	1.98	0.45
1:D:218:THR:HA	1:D:219:PRO:HD3	1.77	0.45
1:E:56:THR:O	1:E:57:GLY:C	2.54	0.45
1:B:66:GLN:O	1:B:70:GLU:HB2	2.16	0.45
1:F:191:SER:HB2	1:F:194:HIS:HB2	1.97	0.45
1:C:214:ILE:HD12	1:C:217:GLU:OE2	2.17	0.45
1:E:158:GLN:HG2	1:G:243:GLN:NE2	2.31	0.45
1:C:37:VAL:HG12	1:C:38:GLU:N	2.30	0.45
1:H:77:GLU:CB	1:H:79:HIS:CD2	2.99	0.45
1:F:165:ASN:HD21	1:F:266:ASP:HA	1.82	0.45
1:C:257:HIS:HD2	4:C:324:HOH:O	1.99	0.45
1:H:42:TYR:HB2	4:H:276:HOH:O	2.16	0.45
1:E:169:TRP:CE2	1:E:256:GLY:HA3	2.51	0.45
1:G:255:VAL:O	1:G:258:HIS:HD2	2.00	0.45
1:D:108:VAL:CG1	1:D:112:LEU:HB3	2.47	0.45
1:G:155:TYR:HB3	1:G:164:MET:HB2	1.99	0.45
1:A:12:SER:HB3	1:A:42:TYR:CE1	2.52	0.45
1:C:49:ILE:HD11	1:D:48:PRO:HG3	1.98	0.45
1:H:70:GLU:OE2	1:H:70:GLU:HA	2.15	0.45
1:C:224:PRO:HD2	1:C:227:LEU:CD2	2.39	0.45
1:C:172:GLN:HG2	1:C:183:VAL:CG1	2.46	0.45
1:E:164:MET:HG3	1:E:164:MET:O	2.17	0.45
1:B:65:PHE:HE1	1:B:70:GLU:HG2	1.81	0.45
1:D:163:ASP:OD2	1:D:165:ASN:HB2	2.16	0.45
1:H:121:ILE:HG22	1:H:122:GLY:N	2.32	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:163:ASP:OD2	1:H:165:ASN:HB2	2.17	0.45
1:H:101:PHE:CZ	1:H:146:ILE:HG12	2.52	0.45
2:C:601:FAD:H2B	2:C:601:FAD:H8A	1.78	0.44
1:F:255:VAL:H	1:F:267:ASN:ND2	2.16	0.44
1:E:25:ALA:O	1:E:29:LEU:HD22	2.17	0.44
1:E:5:ALA:HA	1:E:96:LEU:O	2.17	0.44
1:E:68:PRO:O	1:E:72:VAL:HG23	2.17	0.44
1:C:246:GLU:O	1:C:261:LYS:NZ	2.50	0.44
1:E:127:THR:HG22	1:E:129:ALA:H	1.83	0.44
1:F:150:GLY:HA2	1:F:154:MET:HE1	1.97	0.44
1:F:132:TYR:OH	1:H:161:HIS:CD2	2.58	0.44
2:H:601:FAD:O4	3:H:547:CC2:H11B	2.17	0.44
1:D:71:SER:OG	1:D:121:ILE:HG23	2.17	0.44
1:B:174:GLY:O	1:B:178:PHE:HB2	2.18	0.44
1:G:6:LEU:HD13	1:G:90:LYS:HB3	1.99	0.44
1:E:105:TRP:HB3	1:G:175:ILE:HG12	2.00	0.44
1:B:186:PRO:HB2	1:B:188:LEU:HD21	1.99	0.44
1:D:32:LYS:HD2	1:D:32:LYS:HA	1.82	0.44
1:C:214:ILE:HG23	1:C:215:TRP:N	2.33	0.44
1:B:244:ASP:HA	1:B:247:LYS:HD3	2.00	0.44
3:F:547:CC2:H19	3:F:547:CC2:O7	2.17	0.44
1:F:192:ILE:HA	1:F:192:ILE:HD12	1.87	0.44
1:F:255:VAL:HG23	1:F:267:ASN:HB3	2.00	0.44
1:F:98:ILE:HG12	1:F:143:VAL:CG1	2.48	0.44
1:D:17:PHE:HB2	2:D:601:FAD:H51A	2.00	0.44
1:H:51:SER:O	1:H:54:ASP:HB2	2.17	0.44
1:H:115:TRP:O	1:H:119:VAL:HB	2.18	0.44
1:C:202:GLN:HB3	1:E:202:GLN:HB3	2.00	0.44
1:A:120:PHE:HB3	1:B:105:TRP:CZ2	2.52	0.43
1:C:167:ILE:HD13	1:C:168:LEU:N	2.33	0.43
1:F:157:LEU:O	1:H:259:LEU:HD23	2.18	0.43
1:A:227:LEU:HB3	1:A:242:VAL:HG11	2.00	0.43
1:F:161:HIS:HE1	3:F:547:CC2:O7	2.02	0.43
1:B:194:HIS:HE1	3:B:547:CC2:C21	2.28	0.43
1:F:172:GLN:NE2	4:F:297:HOH:O	2.42	0.43
1:B:58:LYS:N	1:B:58:LYS:HD2	2.32	0.43
1:F:56:THR:HB	1:F:79:HIS:O	2.17	0.43
1:C:257:HIS:HE1	1:D:159:GLY:O	2.01	0.43
1:G:104:GLN:OE1	1:G:109:PRO:HB3	2.18	0.43
1:A:48:PRO:CG	1:B:49:ILE:HD11	2.48	0.43
1:C:75:TYR:CZ	1:C:124:PHE:HB2	2.53	0.43
1:D:12:SER:HB3	1:D:42:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:7:ILE:CG2	1:B:22:LYS:HG2	2.42	0.43
1:H:161:HIS:HE1	3:H:547:CC2:O7	2.02	0.43
1:F:194:HIS:CE1	1:H:232:PHE:HZ	2.36	0.43
1:G:160:ILE:HG13	1:G:160:ILE:O	2.19	0.43
1:H:104:GLN:HA	2:H:601:FAD:C5X	2.49	0.43
1:C:218:THR:HA	1:C:219:PRO:HD3	1.87	0.43
3:E:547:CC2:C8	3:E:547:CC2:H19	2.49	0.43
1:H:72:VAL:HG22	1:H:122:GLY:HA3	2.00	0.43
1:E:262:SER:HA	1:G:261:LYS:O	2.19	0.43
1:H:66:GLN:O	1:H:70:GLU:HB2	2.18	0.43
1:F:196:PRO:O	1:F:199:ALA:HB3	2.19	0.43
1:H:195:THR:O	1:H:196:PRO:C	2.57	0.43
1:C:47:ASN:HA	1:C:48:PRO:HD3	1.89	0.43
1:G:227:LEU:HD23	1:G:242:VAL:HG11	2.01	0.43
1:B:214:ILE:HG23	1:B:215:TRP:N	2.33	0.43
1:H:241:GLU:HG3	1:H:241:GLU:H	1.56	0.43
1:B:147:THR:HG1	2:B:601:FAD:C5'	2.27	0.42
1:A:11:HIS:CE1	1:A:16:SER:HB3	2.54	0.42
1:A:108:VAL:O	1:B:113:LYS:NZ	2.51	0.42
1:A:164:MET:HE1	1:A:168:LEU:HD13	1.97	0.42
1:A:11:HIS:CD2	1:A:18:ASN:HB2	2.54	0.42
1:E:169:TRP:CD1	1:G:166:VAL:HG11	2.54	0.42
1:H:18:ASN:HD22	1:H:100:GLN:HE21	1.66	0.42
1:C:28:ALA:HB2	1:C:208:LYS:HB3	2.01	0.42
1:G:149:GLY:O	1:G:191:SER:HA	2.19	0.42
1:B:126:TYR:HA	1:B:136:PRO:HD2	2.01	0.42
1:C:72:VAL:O	1:C:75:TYR:HB3	2.19	0.42
1:B:155:TYR:HB3	1:B:164:MET:HB2	2.01	0.42
1:A:22:LYS:NZ	1:A:38:GLU:OE2	2.52	0.42
1:F:185:GLU:HA	1:F:186:PRO:HD3	1.85	0.42
1:B:250:LYS:HE2	1:B:251:PHE:CZ	2.55	0.42
1:D:67:TYR:O	1:D:71:SER:CB	2.67	0.42
1:G:85:VAL:O	1:G:89:LYS:HG3	2.19	0.42
1:C:21:MET:HG2	1:C:100:GLN:OE1	2.19	0.42
1:F:5:ALA:HB2	1:F:34:TRP:CE3	2.54	0.42
1:G:29:LEU:HB3	1:G:34:TRP:HB2	2.02	0.42
1:H:35:GLU:HG2	1:H:36:VAL:N	2.34	0.42
1:H:104:GLN:HA	2:H:601:FAD:N5	2.35	0.42
1:H:18:ASN:HD22	1:H:100:GLN:HG3	1.84	0.42
3:D:547:CC2:C8	3:D:547:CC2:H19	2.45	0.42
1:D:132:TYR:CD1	1:D:178:PHE:HA	2.54	0.42
1:C:91:LEU:HA	1:C:91:LEU:HD13	1.76	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:182:GLN:HE21	1:C:219:PRO:HG2	1.85	0.42
1:H:195:THR:HG22	1:H:199:ALA:HB3	2.02	0.42
1:H:25:ALA:O	1:H:29:LEU:HD22	2.19	0.42
1:E:118:ARG:O	1:E:121:ILE:HD11	2.19	0.42
1:F:127:THR:HG22	1:F:129:ALA:H	1.85	0.42
1:G:229:ASP:OD1	1:G:239:LYS:HG2	2.20	0.42
1:E:75:TYR:CE1	1:E:124:PHE:HB2	2.53	0.42
1:E:65:PHE:CE1	1:E:70:GLU:HG3	2.55	0.42
1:E:91:LEU:HD21	1:E:120:PHE:HE1	1.85	0.42
1:F:195:THR:HA	1:F:196:PRO:HD3	1.78	0.42
1:D:270:LYS:HD3	1:D:270:LYS:HA	1.83	0.42
1:B:11:HIS:CE1	1:B:16:SER:HB3	2.54	0.42
1:F:172:GLN:HA	1:F:176:LEU:HD12	2.02	0.42
1:D:132:TYR:O	1:D:134:LYS:N	2.52	0.42
1:D:25:ALA:O	1:D:29:LEU:CD2	2.68	0.42
1:A:96:LEU:HD12	1:A:97:VAL:H	1.85	0.42
3:F:547:CC2:H13	3:F:547:CC2:H20	1.67	0.42
1:A:116:PHE:O	1:A:120:PHE:HB2	2.19	0.42
1:B:141:LYS:HE3	1:B:215:TRP:CD2	2.55	0.42
1:A:235:GLY:O	1:A:236:PHE:HB2	2.20	0.42
1:E:200:ARG:O	1:E:204:LEU:HD22	2.19	0.42
1:H:122:GLY:O	1:H:123:GLU:CB	2.68	0.42
1:C:47:ASN:O	1:C:118:ARG:HD3	2.19	0.42
1:B:255:VAL:H	1:B:267:ASN:ND2	2.17	0.42
1:A:254:SER:HB2	1:A:257:HIS:H	1.85	0.42
3:E:547:CC2:H20	3:E:547:CC2:H13	1.75	0.42
1:G:227:LEU:HG	1:G:242:VAL:HG21	2.02	0.41
1:G:88:GLN:HG2	1:G:124:PHE:CE2	2.54	0.41
1:F:220:LEU:HD21	1:F:268:GLN:O	2.20	0.41
1:D:100:GLN:O	1:D:101:PHE:HB3	2.19	0.41
1:D:224:PRO:HD2	1:D:227:LEU:HD22	2.02	0.41
1:H:48:PRO:O	1:H:114:GLY:HA3	2.20	0.41
1:D:37:VAL:HG21	4:D:338:HOH:O	2.19	0.41
1:G:207:TRP:O	1:G:211:LEU:HG	2.20	0.41
1:F:161:HIS:HD2	1:H:132:TYR:OH	2.01	0.41
1:H:255:VAL:H	1:H:267:ASN:ND2	2.18	0.41
1:A:220:LEU:HD12	1:A:220:LEU:HA	1.87	0.41
1:G:132:TYR:O	1:G:180:GLY:HA2	2.19	0.41
1:D:25:ALA:HB2	1:D:207:TRP:HE1	1.86	0.41
1:E:125:ALA:O	1:E:179:CYS:HB3	2.20	0.41
1:F:30:LYS:NZ	1:F:36:VAL:HB	2.35	0.41
1:B:28:ALA:HB2	1:B:208:LYS:HE3	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:60:LYS:HD2	1:G:73:LEU:HD22	2.01	0.41
1:B:102:PRO:HB3	2:B:601:FAD:H5'1	2.02	0.41
1:E:88:GLN:HG2	1:E:124:PHE:CE2	2.55	0.41
1:C:199:ALA:O	1:C:202:GLN:HB2	2.20	0.41
1:D:108:VAL:HA	1:D:109:PRO:HD3	1.96	0.41
1:E:122:GLY:O	1:E:123:GLU:CB	2.69	0.41
1:F:81:SER:HA	1:F:82:PRO:HD2	1.77	0.41
1:E:131:MET:CE	1:E:178:PHE:CE1	3.03	0.41
1:F:47:ASN:HB3	1:F:118:ARG:NH1	2.36	0.41
1:D:29:LEU:CD2	1:D:211:LEU:HG	2.51	0.41
1:H:189:THR:HG21	1:H:192:ILE:HD13	2.01	0.41
1:D:241:GLU:O	1:D:245:GLU:HG3	2.21	0.41
1:F:130:ALA:HB1	1:F:134:LYS:HB2	2.01	0.41
1:B:17:PHE:CZ	1:B:204:LEU:HD13	2.56	0.41
1:A:132:TYR:CD1	1:A:178:PHE:HA	2.55	0.41
1:C:149:GLY:N	2:C:601:FAD:H2'	2.34	0.41
1:F:28:ALA:HB2	1:F:208:LYS:HE3	2.01	0.41
1:D:148:THR:CG2	1:D:149:GLY:N	2.83	0.41
1:A:41:LEU:HD23	1:A:44:MET:HE1	2.01	0.41
1:F:267:ASN:ND2	1:F:268:GLN:HE21	2.19	0.41
3:C:547:CC2:H20	3:C:547:CC2:H13	1.78	0.41
1:F:238:MET:HB3	1:F:238:MET:HE3	1.82	0.41
1:A:164:MET:CE	1:A:164:MET:O	2.69	0.41
1:E:132:TYR:CD1	1:E:178:PHE:HA	2.56	0.41
1:D:163:ASP:CG	1:D:165:ASN:HB2	2.41	0.41
1:A:218:THR:HA	1:A:219:PRO:HD3	1.79	0.41
1:B:47:ASN:HA	1:B:48:PRO:HD3	1.58	0.41
1:A:58:LYS:O	1:A:58:LYS:HE2	2.19	0.41
1:D:189:THR:CG2	1:D:192:ILE:HD13	2.51	0.41
1:H:211:LEU:HA	1:H:214:ILE:HB	2.01	0.41
1:B:96:LEU:HA	1:B:141:LYS:O	2.21	0.41
1:B:204:LEU:HD12	1:B:204:LEU:HA	1.79	0.41
1:A:164:MET:HG3	1:A:164:MET:O	2.20	0.41
1:A:102:PRO:HB3	2:A:601:FAD:H5'1	2.02	0.41
1:H:148:THR:HG21	1:H:190:TYR:HD1	1.86	0.41
1:F:164:MET:O	1:F:164:MET:CG	2.69	0.41
1:B:186:PRO:HB2	1:B:188:LEU:CD2	2.51	0.41
1:E:50:ILE:HG22	1:E:118:ARG:HG2	2.02	0.41
1:F:11:HIS:CD2	1:F:102:PRO:HG3	2.56	0.41
1:D:249:LYS:NZ	4:D:309:HOH:O	2.54	0.41
1:C:200:ARG:HA	1:C:203:ILE:HD12	2.02	0.41
1:H:97:VAL:HG12	1:H:99:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:17:PHE:H	2:F:601:FAD:C5B	2.34	0.41
2:B:601:FAD:H8A	2:B:601:FAD:H2B	1.91	0.41
1:E:58:LYS:H	1:E:58:LYS:CD	2.28	0.41
1:H:214:ILE:O	1:H:217:GLU:HG3	2.20	0.41
1:C:187:GLN:HG2	1:C:207:TRP:CE3	2.56	0.41
3:C:547:CC2:C17	1:D:128:TYR:HB3	2.51	0.41
1:G:46:PHE:CE2	1:G:47:ASN:O	2.74	0.40
2:H:601:FAD:H2B	2:H:601:FAD:H8A	1.96	0.40
1:F:47:ASN:HA	1:F:48:PRO:HD3	1.81	0.40
1:D:29:LEU:HD12	1:D:34:TRP:CG	2.57	0.40
1:A:238:MET:HB3	1:A:243:GLN:CG	2.51	0.40
1:E:44:MET:HE1	1:E:90:LYS:NZ	2.36	0.40
1:E:121:ILE:HG22	1:E:122:GLY:N	2.36	0.40
1:G:76:LYS:C	1:G:78:GLY:H	2.24	0.40
1:E:238:MET:HB3	1:E:243:GLN:HG2	2.03	0.40
1:A:155:TYR:HB3	1:A:164:MET:HB2	2.03	0.40
1:C:108:VAL:HG13	1:C:112:LEU:HB3	2.03	0.40
1:C:195:THR:HA	1:C:196:PRO:HD3	1.87	0.40
1:F:22:LYS:HG3	1:F:23:GLU:N	2.36	0.40
1:A:52:ARG:H	1:A:52:ARG:HG2	1.58	0.40
1:H:223:ALA:HA	1:H:224:PRO:HD3	1.88	0.40
1:E:189:THR:HG22	1:E:192:ILE:HG12	2.03	0.40
1:F:238:MET:HE3	1:F:242:VAL:HG12	2.03	0.40
1:H:59:LEU:O	1:H:62:PRO:HD3	2.21	0.40
1:A:91:LEU:HA	1:A:91:LEU:HD12	1.75	0.40
1:B:60:LYS:NZ	1:F:240:LYS:HE3	2.36	0.40
1:G:255:VAL:H	1:G:267:ASN:ND2	2.18	0.40
1:H:202:GLN:O	1:H:205:GLU:HB2	2.22	0.40
1:G:108:VAL:HG13	1:G:112:LEU:HB3	2.04	0.40
1:G:229:ASP:O	1:G:236:PHE:HA	2.22	0.40
1:C:81:SER:HA	1:C:82:PRO:HD3	1.94	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

There are no protein chains in this entry.

### 5.3.2 Protein sidechains ⓘ

There are no protein chains in this entry.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

16 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	$\# Z  > 2$
3	CC2	A	547	-	28,28,28	1.68	2 (7%)	39,41,41	3.07	7 (17%)
2	FAD	A	601	-	58,58,58	0.99	3 (5%)	85,89,89	2.79	19 (22%)
3	CC2	B	547	-	28,28,28	1.98	1 (3%)	39,41,41	2.85	6 (15%)
2	FAD	B	601	-	58,58,58	1.05	4 (6%)	85,89,89	2.54	22 (25%)
3	CC2	C	547	-	28,28,28	1.57	1 (3%)	39,41,41	3.06	6 (15%)
2	FAD	C	601	-	58,58,58	1.10	5 (8%)	85,89,89	2.48	19 (22%)
3	CC2	D	547	-	28,28,28	1.97	1 (3%)	39,41,41	2.63	4 (10%)
2	FAD	D	601	-	58,58,58	1.12	4 (6%)	85,89,89	2.47	21 (24%)
3	CC2	E	547	-	28,28,28	1.79	1 (3%)	39,41,41	3.86	5 (12%)
2	FAD	E	601	-	58,58,58	0.96	3 (5%)	85,89,89	2.14	16 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	CC2	F	547	-	28,28,28	1.71	1 (3%)	39,41,41	3.41	5 (12%)
2	FAD	F	601	-	58,58,58	1.04	4 (6%)	85,89,89	2.38	17 (20%)
3	CC2	G	547	-	28,28,28	1.46	2 (7%)	39,41,41	3.58	6 (15%)
2	FAD	G	601	-	58,58,58	0.99	3 (5%)	85,89,89	2.60	22 (25%)
3	CC2	H	547	-	28,28,28	2.05	1 (3%)	39,41,41	4.40	7 (17%)
2	FAD	H	601	-	58,58,58	1.07	4 (6%)	85,89,89	2.48	17 (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
3	CC2	A	547	-	-	0/4/4/4	0/0/4/4
2	FAD	A	601	-	-	0/34/50/50	0/1/6/6
3	CC2	B	547	-	-	0/4/4/4	0/0/4/4
2	FAD	B	601	-	-	0/34/50/50	0/1/6/6
3	CC2	C	547	-	-	0/4/4/4	0/0/4/4
2	FAD	C	601	-	-	0/34/50/50	0/1/6/6
3	CC2	D	547	-	-	0/4/4/4	0/0/4/4
2	FAD	D	601	-	-	0/34/50/50	0/1/6/6
3	CC2	E	547	-	-	0/4/4/4	0/0/4/4
2	FAD	E	601	-	-	0/34/50/50	0/1/6/6
3	CC2	F	547	-	-	0/4/4/4	0/0/4/4
2	FAD	F	601	-	-	0/34/50/50	0/1/6/6
3	CC2	G	547	-	-	0/4/4/4	0/0/4/4
2	FAD	G	601	-	-	0/34/50/50	0/1/6/6
3	CC2	H	547	-	-	0/4/4/4	0/0/4/4
2	FAD	H	601	-	-	0/34/50/50	0/1/6/6

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	547	CC2	O2-C8	9.33	1.37	1.33
3	B	547	CC2	O2-C8	9.31	1.37	1.33
3	D	547	CC2	O2-C8	9.20	1.37	1.33
3	E	547	CC2	O2-C8	8.08	1.37	1.33
3	F	547	CC2	O2-C8	7.56	1.37	1.33
3	A	547	CC2	O2-C8	6.85	1.36	1.33
3	C	547	CC2	O2-C8	6.60	1.36	1.33
3	G	547	CC2	O2-C8	5.82	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FAD	C1'-N10	4.03	1.52	1.48
2	D	601	FAD	C2A-N3A	3.45	1.39	1.32
2	F	601	FAD	C1'-N10	3.41	1.52	1.48
2	A	601	FAD	C2A-N3A	3.28	1.38	1.32
2	H	601	FAD	C2A-N3A	3.24	1.38	1.32
2	C	601	FAD	C2A-N3A	3.11	1.38	1.32
2	G	601	FAD	C1'-N10	3.08	1.51	1.48
2	B	601	FAD	C2A-N3A	3.07	1.38	1.32
2	G	601	FAD	C2A-N3A	3.06	1.38	1.32
2	E	601	FAD	C2A-N3A	2.97	1.38	1.32
2	F	601	FAD	C2A-N3A	2.96	1.38	1.32
2	D	601	FAD	C2A-N1A	2.79	1.39	1.33
2	H	601	FAD	C1'-N10	2.79	1.51	1.48
2	B	601	FAD	C1'-N10	2.78	1.51	1.48
2	A	601	FAD	C2A-N1A	2.69	1.39	1.33
2	C	601	FAD	C1'-C2'	-2.60	1.49	1.51
2	C	601	FAD	C6-C5X	-2.59	1.38	1.41
2	C	601	FAD	C1'-N10	2.55	1.51	1.48
2	C	601	FAD	C2A-N1A	2.50	1.38	1.33
2	A	601	FAD	C6-C5X	-2.32	1.39	1.41
2	H	601	FAD	C2A-N1A	2.30	1.38	1.33
2	B	601	FAD	C2A-N1A	2.29	1.38	1.33
2	H	601	FAD	C6-C5X	-2.25	1.39	1.41
2	E	601	FAD	C1'-N10	2.21	1.50	1.48
2	B	601	FAD	C4'-C3'	-2.20	1.48	1.53
2	E	601	FAD	C2A-N1A	2.17	1.38	1.33
2	F	601	FAD	C6-C5X	-2.16	1.39	1.41
2	F	601	FAD	C2A-N1A	2.11	1.38	1.33
2	D	601	FAD	C5X-N5	2.09	1.38	1.35
3	A	547	CC2	C4-C3	-2.08	1.38	1.41
3	G	547	CC2	C15-C16	-2.08	1.39	1.42
2	G	601	FAD	C2A-N1A	2.03	1.37	1.33

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	547	CC2	O2-C8-C9	-22.30	118.67	125.82
3	E	547	CC2	O2-C8-C9	-20.40	119.28	125.82
3	G	547	CC2	O2-C8-C9	-18.98	119.74	125.82
3	F	547	CC2	O2-C8-C9	-17.63	120.17	125.82
3	C	547	CC2	O2-C8-C9	-15.99	120.70	125.82
3	B	547	CC2	O2-C8-C9	-14.16	121.28	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	547	CC2	O2-C8-C9	-14.16	121.28	125.82
2	A	601	FAD	C1'-N10-C9A	-13.75	105.50	118.87
3	H	547	CC2	C8-O2-C3	13.23	122.61	118.14
3	D	547	CC2	O2-C8-C9	-12.17	121.92	125.82
2	C	601	FAD	C1'-N10-C10	-11.26	103.18	119.17
2	G	601	FAD	C1'-N10-C9A	-10.95	108.22	118.87
2	C	601	FAD	N3A-C2A-N1A	-10.48	119.95	128.71
2	H	601	FAD	N3A-C2A-N1A	-10.42	120.00	128.71
2	B	601	FAD	C1'-N10-C10	-10.33	104.51	119.17
2	B	601	FAD	N3A-C2A-N1A	-10.20	120.18	128.71
2	E	601	FAD	N3A-C2A-N1A	-10.18	120.20	128.71
2	G	601	FAD	N3A-C2A-N1A	-10.13	120.24	128.71
2	F	601	FAD	N3A-C2A-N1A	-10.02	120.34	128.71
3	E	547	CC2	C8-O2-C3	9.95	121.50	118.14
2	A	601	FAD	N3A-C2A-N1A	-9.93	120.41	128.71
2	D	601	FAD	C1'-N10-C10	-9.86	105.18	119.17
2	D	601	FAD	N3A-C2A-N1A	-9.23	120.99	128.71
2	F	601	FAD	C1'-N10-C9A	-9.07	110.05	118.87
2	E	601	FAD	C1'-N10-C10	-8.94	106.48	119.17
3	A	547	CC2	C8-O2-C3	8.90	121.15	118.14
2	H	601	FAD	C1'-N10-C9A	-8.75	110.36	118.87
2	A	601	FAD	C1'-N10-C10	-8.30	107.38	119.17
3	F	547	CC2	C8-O2-C3	8.19	120.91	118.14
2	G	601	FAD	C1'-N10-C10	-8.11	107.66	119.17
3	G	547	CC2	C8-O2-C3	8.07	120.87	118.14
2	C	601	FAD	C1'-N10-C9A	-8.06	111.03	118.87
2	H	601	FAD	C1'-N10-C10	-8.06	107.73	119.17
2	B	601	FAD	C1'-N10-C9A	-7.95	111.14	118.87
2	F	601	FAD	C1'-N10-C10	-7.70	108.24	119.17
2	G	601	FAD	O4B-C1B-N9A	7.02	114.97	108.44
2	A	601	FAD	C2-N1-C10	6.89	121.92	114.98
3	D	547	CC2	C8-O2-C3	6.86	120.46	118.14
2	B	601	FAD	C2-N1-C10	6.60	121.63	114.98
3	B	547	CC2	C1-C2-C3	-6.59	119.64	123.23
3	C	547	CC2	C8-O2-C3	6.57	120.36	118.14
2	D	601	FAD	C1'-N10-C9A	-6.46	112.59	118.87
2	A	601	FAD	C2'-C1'-N10	6.30	120.81	112.45
3	A	547	CC2	C1-C2-C3	-6.22	119.84	123.23
2	H	601	FAD	C2-N1-C10	6.12	121.15	114.98
2	F	601	FAD	C2-N1-C10	6.12	121.14	114.98
3	F	547	CC2	C1-C2-C3	-5.89	120.02	123.23
2	D	601	FAD	C2-N1-C10	5.86	120.89	114.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	FAD	C2-N1-C10	5.81	120.83	114.98
2	D	601	FAD	O4B-C1B-N9A	5.73	113.77	108.44
2	C	601	FAD	C2-N1-C10	5.73	120.75	114.98
2	H	601	FAD	C2'-C1'-N10	5.65	119.95	112.45
2	E	601	FAD	C2-N1-C10	5.58	120.60	114.98
3	B	547	CC2	C8-O2-C3	5.55	120.02	118.14
2	D	601	FAD	C9A-N10-C10	-5.50	116.36	121.77
3	D	547	CC2	C1-C2-C3	-5.35	120.32	123.23
2	B	601	FAD	C4X-C10-N1	-5.33	117.40	122.73
3	E	547	CC2	C1-C2-C3	-5.30	120.35	123.23
2	H	601	FAD	C9A-N10-C10	-5.27	116.60	121.77
2	C	601	FAD	C9A-N10-C10	-5.26	116.61	121.77
3	H	547	CC2	C1-C2-C3	-5.21	120.39	123.23
3	C	547	CC2	C1-C2-C3	-5.11	120.45	123.23
2	A	601	FAD	C1'-C2'-C3'	-5.02	95.45	109.82
2	G	601	FAD	C9A-N10-C10	-4.95	116.91	121.77
2	B	601	FAD	C9A-N10-C10	-4.94	116.92	121.77
2	E	601	FAD	C1'-N10-C9A	-4.92	114.09	118.87
2	F	601	FAD	C4X-C10-N1	-4.89	117.85	122.73
2	H	601	FAD	C4X-C10-N1	-4.86	117.88	122.73
2	F	601	FAD	C9A-N10-C10	-4.84	117.02	121.77
2	D	601	FAD	C5X-C9A-N10	4.82	121.55	116.80
3	G	547	CC2	C1-C2-C3	-4.74	120.65	123.23
2	G	601	FAD	C4X-C10-N1	-4.71	118.03	122.73
2	A	601	FAD	C4X-C10-N1	-4.69	118.04	122.73
2	H	601	FAD	O4B-C1B-N9A	4.63	112.75	108.44
2	G	601	FAD	C2'-C1'-N10	4.47	118.38	112.45
2	A	601	FAD	C9A-N10-C10	-4.37	117.48	121.77
2	H	601	FAD	C5X-C9A-N10	4.27	121.00	116.80
2	G	601	FAD	C5X-C9A-N10	4.26	121.00	116.80
3	H	547	CC2	O2-C3-C2	4.17	121.27	115.90
2	F	601	FAD	O4B-C1B-N9A	3.95	112.11	108.44
2	D	601	FAD	C2'-C1'-N10	3.91	117.64	112.45
2	A	601	FAD	N3A-C4A-N9A	3.87	132.43	125.43
2	C	601	FAD	C5X-C9A-N10	3.86	120.60	116.80
2	C	601	FAD	C4X-C10-N1	-3.84	118.89	122.73
2	E	601	FAD	C9A-N10-C10	-3.80	118.04	121.77
2	C	601	FAD	N3A-C4A-N9A	3.74	132.18	125.43
2	D	601	FAD	N3A-C4A-N9A	3.72	132.15	125.43
2	A	601	FAD	C5X-C9A-N10	3.69	120.44	116.80
2	D	601	FAD	C4X-C10-N1	-3.61	119.12	122.73
2	F	601	FAD	C5X-C9A-N10	3.60	120.34	116.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	FAD	C5X-C9A-N10	3.56	120.31	116.80
2	F	601	FAD	C2'-C1'-N10	3.45	117.03	112.45
2	F	601	FAD	N3A-C4A-N9A	3.44	131.64	125.43
2	E	601	FAD	N3A-C4A-N9A	3.41	131.58	125.43
3	G	547	CC2	O1-C10-C4	3.33	123.02	116.55
2	F	601	FAD	C4X-N5-C5X	3.32	120.42	116.69
2	B	601	FAD	N3A-C4A-N9A	3.31	131.42	125.43
2	B	601	FAD	C2'-C1'-N10	3.30	116.83	112.45
2	B	601	FAD	C5X-C9A-N10	3.25	120.00	116.80
2	B	601	FAD	C4X-N5-C5X	3.24	120.33	116.69
2	E	601	FAD	C4X-C10-N1	-3.15	119.58	122.73
2	G	601	FAD	N3A-C4A-N9A	3.15	131.12	125.43
2	D	601	FAD	C5'-C4'-C3'	-3.13	106.15	112.06
2	E	601	FAD	C4X-N5-C5X	3.08	120.15	116.69
2	B	601	FAD	O4B-C1B-N9A	-3.08	105.58	108.44
2	B	601	FAD	C4-N3-C2	-3.06	119.11	125.39
2	F	601	FAD	C4X-C10-N10	3.05	122.03	120.51
2	G	601	FAD	C4X-N5-C5X	3.03	120.10	116.69
2	A	601	FAD	O4'-C4'-C5'	-3.01	103.93	110.12
2	D	601	FAD	C4X-C10-N10	3.00	122.01	120.51
2	H	601	FAD	N3A-C4A-N9A	2.99	130.84	125.43
3	H	547	CC2	C5-C4-C3	2.99	119.96	116.30
3	D	547	CC2	O2-C3-C2	2.97	119.72	115.90
3	H	547	CC2	C2-C3-C4	-2.96	119.49	123.10
2	A	601	FAD	O3'-C3'-C4'	2.95	116.19	108.74
2	F	601	FAD	C4-N3-C2	-2.92	119.39	125.39
3	A	547	CC2	O2-C3-C2	2.89	119.62	115.90
2	G	601	FAD	C4A-C5A-N7A	-2.83	107.10	109.52
2	B	601	FAD	C4A-C5A-N7A	-2.81	107.11	109.52
2	A	601	FAD	O2'-C2'-C1'	2.80	116.67	109.71
2	D	601	FAD	O3'-C3'-C2'	2.80	115.80	108.74
2	B	601	FAD	C4X-C10-N10	2.78	121.90	120.51
2	F	601	FAD	C4-C4X-C10	2.77	121.42	116.95
2	C	601	FAD	C4-N3-C2	-2.76	119.72	125.39
2	D	601	FAD	P-O3P-PA	-2.76	123.58	131.68
3	C	547	CC2	C5-C4-C3	2.75	119.66	116.30
2	G	601	FAD	C5'-C4'-C3'	-2.70	106.97	112.06
2	H	601	FAD	C4-N3-C2	-2.69	119.87	125.39
2	A	601	FAD	O4B-C1B-N9A	2.67	110.92	108.44
2	B	601	FAD	C4'-C3'-C2'	-2.65	107.25	113.25
2	A	601	FAD	C4-N3-C2	-2.64	119.98	125.39
2	G	601	FAD	C4-N3-C2	-2.59	120.07	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	FAD	C4-N3-C2	-2.59	120.08	125.39
2	A	601	FAD	C4X-N5-C5X	2.58	119.59	116.69
2	D	601	FAD	C4X-N5-C5X	2.53	119.54	116.69
3	B	547	CC2	C5-C4-C3	2.52	119.39	116.30
2	G	601	FAD	C4X-C10-N10	2.52	121.76	120.51
2	B	601	FAD	C4-C4X-C10	2.51	121.00	116.95
2	H	601	FAD	O2A-PA-O3P	2.51	117.03	105.14
2	G	601	FAD	C4-C4X-C10	2.50	120.99	116.95
2	E	601	FAD	C8A-N9A-C4A	2.50	108.81	106.90
3	A	547	CC2	C14-C13-C9	-2.48	106.75	114.11
2	H	601	FAD	C4A-C5A-N7A	-2.45	107.42	109.52
2	C	601	FAD	N7A-C8A-N9A	-2.44	107.44	114.36
2	C	601	FAD	C4X-C10-N10	2.44	121.72	120.51
2	C	601	FAD	C5B-C4B-C3B	-2.42	105.50	115.21
2	E	601	FAD	N7A-C8A-N9A	-2.42	107.51	114.36
2	C	601	FAD	O4B-C1B-N9A	-2.42	106.19	108.44
2	H	601	FAD	N7A-C8A-N9A	-2.40	107.56	114.36
2	B	601	FAD	O4'-C4'-C3'	-2.39	103.09	109.05
2	D	601	FAD	O3'-C3'-C4'	-2.38	102.71	108.74
2	G	601	FAD	O2A-PA-O3P	2.38	116.41	105.14
2	H	601	FAD	C4-C4X-C10	2.37	120.78	116.95
2	D	601	FAD	C4-N3-C2	-2.35	120.56	125.39
3	C	547	CC2	C2-C3-C4	-2.35	120.22	123.10
2	B	601	FAD	N7A-C8A-N9A	-2.35	107.71	114.36
2	H	601	FAD	C4X-C10-N10	2.34	121.68	120.51
3	G	547	CC2	C14-C13-C9	-2.34	107.16	114.11
2	A	601	FAD	C5A-C4A-N3A	-2.33	120.62	125.70
2	B	601	FAD	C6-C5X-C9A	2.32	122.22	119.02
2	E	601	FAD	C4X-C10-N10	2.31	121.66	120.51
2	G	601	FAD	N7A-C8A-N9A	-2.28	107.92	114.36
3	F	547	CC2	O1-C10-C4	2.27	120.96	116.55
2	D	601	FAD	C5A-C4A-N3A	-2.25	120.80	125.70
3	B	547	CC2	O2-C3-C2	2.25	118.80	115.90
2	D	601	FAD	O5B-PA-O1A	2.24	118.16	109.37
3	F	547	CC2	O2-C3-C2	2.24	118.78	115.90
3	C	547	CC2	O2-C3-C2	2.24	118.78	115.90
2	C	601	FAD	C5A-C4A-N3A	-2.23	120.85	125.70
2	A	601	FAD	O2P-P-O3P	2.22	115.69	105.14
2	B	601	FAD	C5'-C4'-C3'	-2.19	107.92	112.06
2	C	601	FAD	C4-C4X-C10	2.16	120.44	116.95
2	C	601	FAD	C4A-C5A-N7A	-2.16	107.67	109.52
2	B	601	FAD	C5A-C4A-N3A	-2.16	121.00	125.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	FAD	N7A-C8A-N9A	-2.15	108.27	114.36
3	A	547	CC2	C5-C4-C3	2.15	118.93	116.30
2	H	601	FAD	C8A-N9A-C4A	2.14	108.53	106.90
2	G	601	FAD	C5A-C4A-N3A	-2.14	121.04	125.70
2	F	601	FAD	C2B-C1B-N9A	-2.13	107.79	113.27
2	C	601	FAD	C8A-N9A-C4A	2.13	108.52	106.90
2	B	601	FAD	C2A-N3A-C4A	2.12	120.06	114.01
3	E	547	CC2	O2-C3-C2	2.12	118.63	115.90
3	E	547	CC2	O1-C10-C4	2.10	120.63	116.55
2	D	601	FAD	O4'-C4'-C5'	2.10	114.43	110.12
2	E	601	FAD	C5'-C4'-C3'	-2.10	108.11	112.06
2	A	601	FAD	N7A-C8A-N9A	-2.08	108.47	114.36
2	F	601	FAD	C5A-C4A-N3A	-2.07	121.19	125.70
2	G	601	FAD	O2P-P-O3P	2.07	114.95	105.14
3	A	547	CC2	O2-C3-C4	-2.07	119.22	121.36
3	B	547	CC2	C2-C3-C4	-2.06	120.58	123.10
2	F	601	FAD	N7A-C8A-N9A	-2.06	108.54	114.36
2	C	601	FAD	O2A-PA-O3P	2.05	114.87	105.14
3	H	547	CC2	O2-C3-C4	-2.04	119.24	121.36
2	E	601	FAD	C4A-C5A-N7A	-2.03	107.78	109.52
2	E	601	FAD	C2A-N3A-C4A	2.03	119.78	114.01
2	G	601	FAD	C2A-N3A-C4A	2.02	119.75	114.01
2	G	601	FAD	O3'-C3'-C4'	-2.02	103.64	108.74
3	G	547	CC2	C5-C4-C10	2.01	123.69	120.84
2	C	601	FAD	C2A-N3A-C4A	2.00	119.71	114.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	270/273 (98%)	0.16	3 (1%) 77 78	42, 61, 78, 92	0
1	B	270/273 (98%)	0.04	0 100 100	42, 56, 75, 87	0
1	C	270/273 (98%)	0.02	1 (0%) 90 92	41, 57, 75, 91	0
1	D	270/273 (98%)	0.10	2 (0%) 84 86	42, 59, 78, 90	0
1	E	270/273 (98%)	0.17	5 (1%) 64 65	51, 67, 89, 98	0
1	F	270/273 (98%)	0.20	4 (1%) 70 71	50, 66, 87, 102	0
1	G	270/273 (98%)	0.22	5 (1%) 64 65	50, 69, 95, 105	0
1	H	270/273 (98%)	0.34	8 (2%) 48 49	51, 70, 93, 105	0
All	All	2160/2184 (98%)	0.15	28 (1%) 74 75	41, 63, 87, 105	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	2	GLY	9.0
1	F	2	GLY	4.8
1	G	2	GLY	4.7
1	H	59	LEU	3.8
1	A	232	PHE	3.1
1	E	29	LEU	2.8
1	F	209	LYS	2.8
1	G	230	LEU	2.7
1	G	259	LEU	2.7
1	H	73	LEU	2.7
1	D	2	GLY	2.6
1	G	59	LEU	2.6
1	E	10	ALA	2.4
1	E	55	ILE	2.4
1	F	248	ASN	2.3
1	H	251	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	58	LYS	2.3
1	A	7	ILE	2.3
1	D	232	PHE	2.3
1	H	34	TRP	2.2
1	E	160	ILE	2.2
1	H	24	ALA	2.2
1	A	58	LYS	2.1
1	E	80	LEU	2.1
1	G	253	LEU	2.1
1	F	7	ILE	2.1
1	C	2	GLY	2.0
1	H	36	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CC2	F	547	25/25	0.23	1.46	59,68,81,82	0
3	CC2	C	547	25/25	0.21	0.88	52,62,85,89	0
3	CC2	B	547	25/25	0.22	0.71	57,66,87,89	0
3	CC2	E	547	25/25	0.17	0.14	60,68,81,85	0
3	CC2	G	547	25/25	0.17	0.09	53,56,59,60	0
3	CC2	A	547	25/25	0.16	0.06	44,49,53,56	0
2	FAD	B	601	53/53	0.14	-0.17	46,58,66,68	0
2	FAD	F	601	53/53	0.15	-0.29	53,62,69,76	0
2	FAD	H	601	53/53	0.15	-0.38	43,56,69,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	D	601	53/53	0.14	-0.39	42,50,62,68	0
3	CC2	D	547	25/25	0.15	-0.48	46,51,54,55	0
3	CC2	H	547	25/25	0.14	-0.57	51,55,58,60	0
2	FAD	C	601	53/53	0.14	-0.59	39,54,63,69	0
2	FAD	A	601	53/53	0.15	-0.62	42,49,61,64	0
2	FAD	G	601	53/53	0.14	-0.63	42,54,62,68	0
2	FAD	E	601	53/53	0.14	-0.94	56,63,73,80	0

## 6.5 Other polymers

There are no such residues in this entry.