



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 07:21 AM EDT

PDB ID : 9QGZ / pdb_00009qgz
Title : Crystal structure of a D-lactate dehydrogenase from Porcellio dilatatus
Authors : Borges, P.T.; Frazao, C.; Martins, L.O.
Deposited on : 2025-03-14
Resolution : 2.84 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

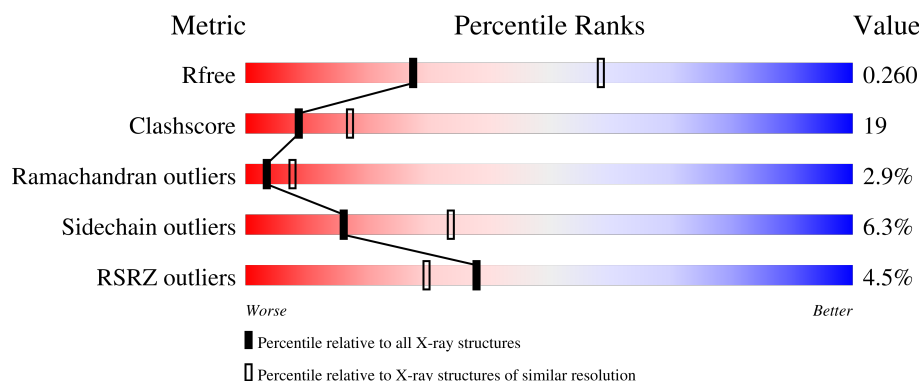
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	464	
1	B	464	
1	C	464	
1	D	464	
1	E	464	

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Mol	Chain	Length	Quality of chain
1	F	464	
1	G	464	
1	H	464	

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
2	FAD	C	501	-	-	X	-
2	FAD	E	501	-	-	X	-
2	FAD	H	501	-	-	X	-

2 Entry composition

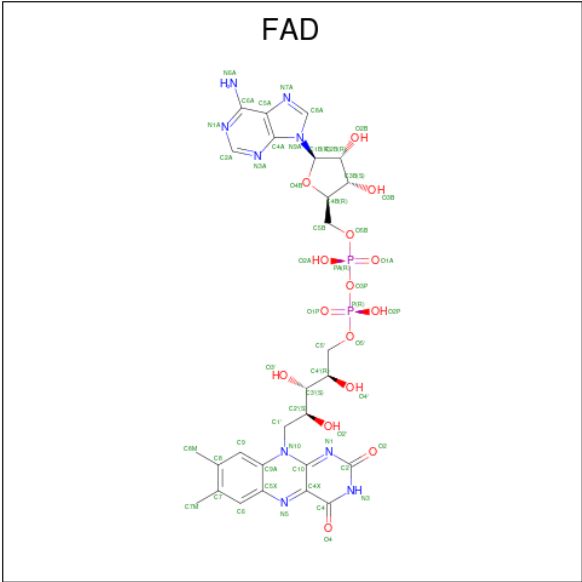
There are 4 unique types of molecules in this entry. The entry contains 26348 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycolate oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3296	2065	585	633	13			
1	B	447	Total	C	N	O	S	0	0	0
			3315	2076	590	635	14			
1	C	445	Total	C	N	O	S	0	0	0
			3305	2067	588	636	14			
1	D	453	Total	C	N	O	S	0	0	0
			3343	2092	591	646	14			
1	E	450	Total	C	N	O	S	0	0	0
			3326	2080	591	642	13			
1	F	444	Total	C	N	O	S	0	0	0
			3273	2047	587	625	14			
1	G	453	Total	C	N	O	S	0	0	0
			3343	2092	591	646	14			
1	H	369	Total	C	N	O	S	0	0	0
			2679	1678	475	515	11			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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 FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	B	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total 1	Fe 1	0	0
3	E	1	Total 1	Fe 1	0	0
3	F	1	Total 1	Fe 1	0	0
3	G	1	Total 1	Fe 1	0	0
3	H	1	Total 1	Fe 1	0	0

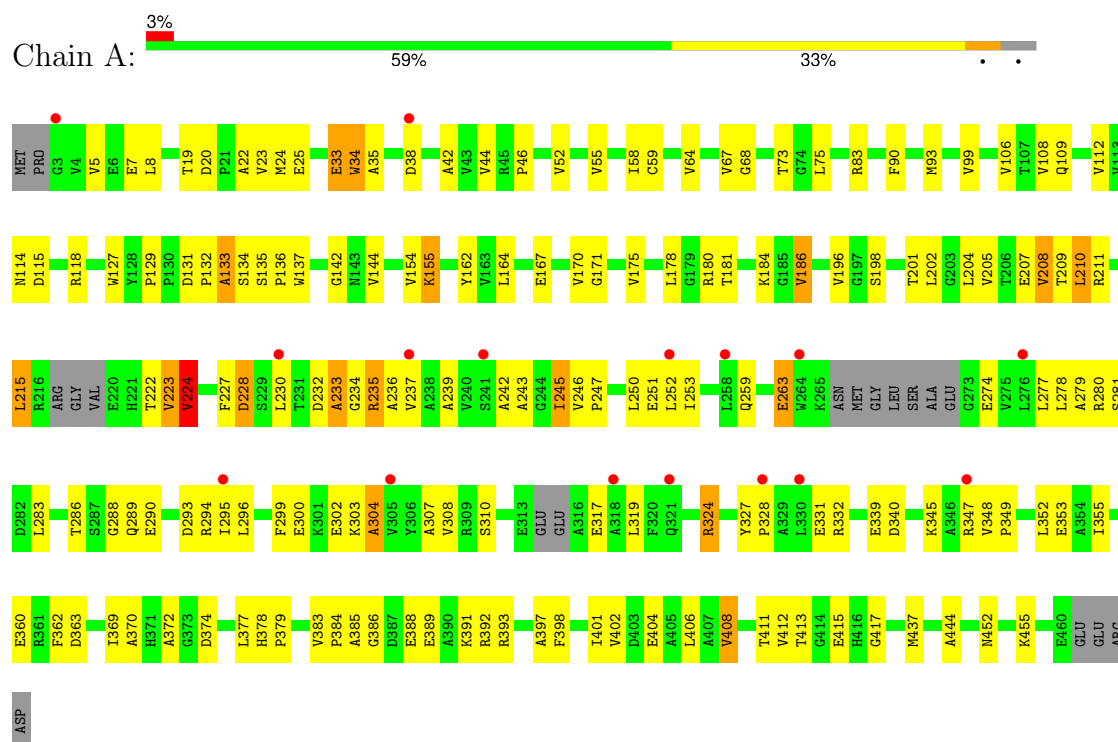
- Molecule 4 is water.

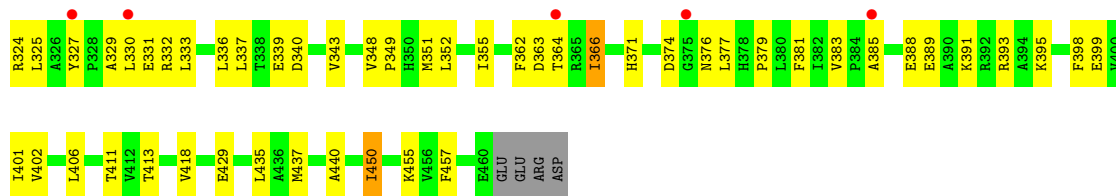
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total 6	O 6	0	0
4	B	3	Total 3	O 3	0	0
4	C	7	Total 7	O 7	0	0
4	D	2	Total 2	O 2	0	0
4	E	3	Total 3	O 3	0	0
4	F	5	Total 5	O 5	0	0
4	G	4	Total 4	O 4	0	0
4	H	6	Total 6	O 6	0	0

3 Residue-property plots [i](#)

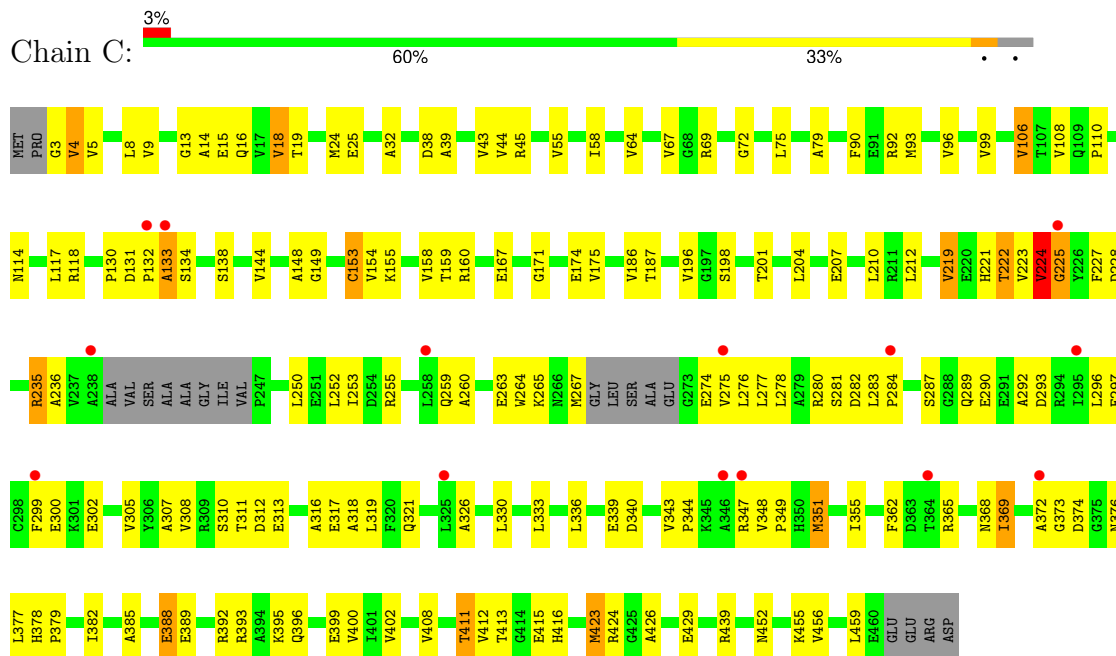
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Glycolate oxidase





• Molecule 1: Glycolate oxidase

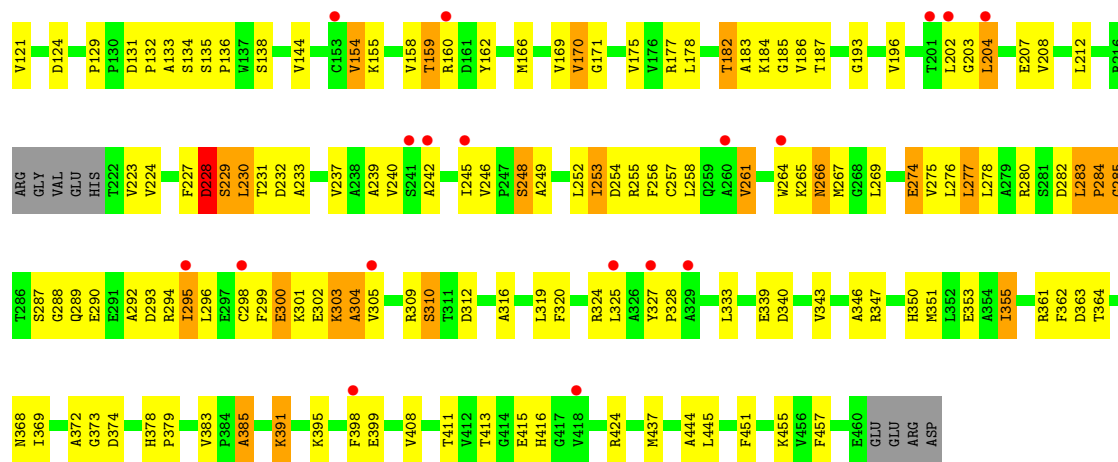


• Molecule 1: Glycolate oxidase

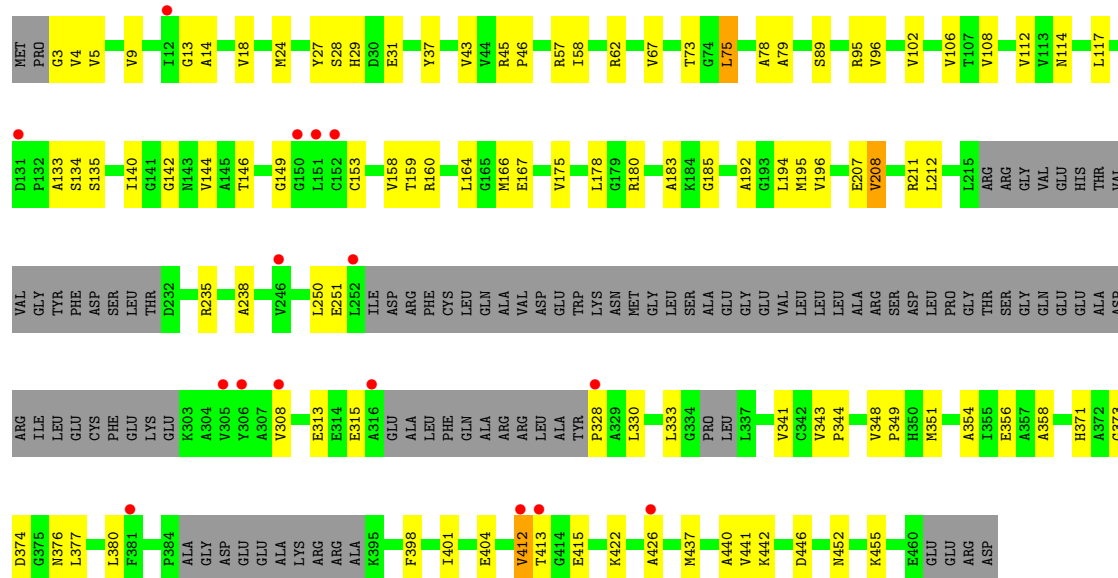


• Molecule 1: Glycolate oxidase





• Molecule 1: Glycolate oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.67Å 103.92Å 143.83Å 81.94° 77.24° 75.41°	Depositor
Resolution (Å)	78.15 – 2.84 78.15 – 2.84	Depositor EDS
% Data completeness (in resolution range)	51.9 (78.15-2.84) 51.9 (78.15-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.207 , 0.262 0.208 , 0.260	Depositor DCC
R_{free} test set	2201 reflections (2.46%)	wwPDB-VP
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	26348	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.18	0/3350	0.50	0/4556
1	B	0.15	0/3368	0.46	0/4578
1	C	0.19	0/3360	0.50	0/4567
1	D	0.20	0/3398	0.50	0/4623
1	E	0.15	0/3381	0.50	0/4599
1	F	0.19	0/3325	0.51	0/4520
1	G	0.19	0/3398	0.48	0/4623
1	H	0.09	0/2720	0.27	0/3702
All	All	0.17	0/26300	0.47	0/35768

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	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	232	ASP	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3296	0	3278	119	0
1	B	3315	0	3299	107	0
1	C	3305	0	3280	136	0
1	D	3343	0	3324	131	1
1	E	3326	0	3299	130	1
1	F	3273	0	3270	139	0
1	G	3343	0	3324	137	0
1	H	2679	0	2673	87	0
2	A	53	0	31	10	0
2	B	53	0	31	7	0
2	C	53	0	31	26	0
2	D	53	0	31	14	0
2	E	53	0	31	30	0
2	F	53	0	31	18	0
2	G	53	0	31	11	0
2	H	53	0	31	33	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	6	0	0	0	0
4	B	3	0	0	0	0
4	C	7	0	0	0	0
4	D	2	0	0	0	0
4	E	3	0	0	0	0
4	F	5	0	0	0	0
4	G	4	0	0	0	0
4	H	6	0	0	0	0
All	All	26348	0	25995	979	1

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 19.

All (979) 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:H:328:PRO:HD3	2:H:501:FAD:C7M	1.55	1.36
1:E:133:ALA:HB3	2:E:501:FAD:N5	1.44	1.31
1:H:133:ALA:HB3	2:H:501:FAD:N5	1.47	1.25
1:C:110:PRO:CB	2:C:501:FAD:N6A	2.00	1.23
1:E:73:THR:OG1	2:E:501:FAD:O2P	1.63	1.13
1:G:160:ARG:HH12	1:G:193:GLY:HA2	1.13	1.12
1:C:110:PRO:CB	2:C:501:FAD:H61A	1.58	1.12
1:C:110:PRO:HB3	2:C:501:FAD:N6A	1.63	1.11
1:E:138:SER:OG	2:E:501:FAD:H4'	1.50	1.10
1:D:327:TYR:HD2	2:D:501:FAD:HM73	1.07	1.08
1:D:216:ARG:HH22	1:D:282:ASP:HB2	1.17	1.08
1:E:138:SER:CB	2:E:501:FAD:H4'	1.84	1.08
1:F:328:PRO:HD3	2:F:501:FAD:HM71	1.34	1.08
1:C:110:PRO:HB2	2:C:501:FAD:H61A	0.94	1.06
1:H:134:SER:OG	2:H:501:FAD:C9	2.04	1.06
2:D:501:FAD:H8A	2:D:501:FAD:H51A	1.34	1.05
1:H:328:PRO:HD3	2:H:501:FAD:HM71	1.38	1.04
1:F:133:ALA:HB3	2:F:501:FAD:N5	1.72	1.03
1:D:327:TYR:HD2	2:D:501:FAD:C7M	1.77	0.98
1:D:327:TYR:CD2	2:D:501:FAD:HM73	1.98	0.98
1:C:110:PRO:HB2	2:C:501:FAD:N6A	1.70	0.96
1:D:378:HIS:NE2	1:D:415:GLU:OE2	1.99	0.95
1:D:123:GLN:HB3	1:E:235:ARG:HH21	1.32	0.94
1:A:362:PHE:HB3	1:A:393:ARG:HB3	1.47	0.94
1:E:138:SER:OG	2:E:501:FAD:C4'	2.14	0.94
1:F:363:ASP:HB3	1:F:393:ARG:HH22	1.34	0.93
1:H:328:PRO:HD3	2:H:501:FAD:HM72	1.50	0.92
1:H:134:SER:OG	2:H:501:FAD:C9A	2.18	0.91
1:D:259:GLN:NE2	1:D:263:GLU:OE2	2.04	0.90
1:G:228:ASP:HB3	1:G:274:GLU:H	1.35	0.89
1:D:123:GLN:HB3	1:E:235:ARG:NH2	1.87	0.89
1:H:133:ALA:HB3	2:H:501:FAD:C5X	2.04	0.88
1:E:73:THR:O	2:E:501:FAD:H9	1.74	0.88
1:C:110:PRO:HB3	2:C:501:FAD:H62A	1.36	0.88
1:F:328:PRO:HD3	2:F:501:FAD:C7M	2.04	0.87
2:D:501:FAD:H51A	2:D:501:FAD:C8A	2.04	0.86
1:G:253:ILE:HD11	1:G:257:CYS:HB2	1.55	0.85
1:H:134:SER:HG	2:H:501:FAD:C9	1.91	0.84
1:G:231:THR:HG23	1:G:353:GLU:HG2	1.59	0.84
1:E:138:SER:HB2	2:E:501:FAD:H4'	1.57	0.83
1:H:73:THR:HG23	2:H:501:FAD:O3'	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:9:VAL:HA	1:H:13:GLY:HA3	1.61	0.82
1:H:133:ALA:CB	2:H:501:FAD:H6	2.10	0.82
1:A:33:GLU:O	1:A:35:ALA:N	2.12	0.81
1:A:142:GLY:HA3	2:A:501:FAD:O1P	1.78	0.81
1:B:97:LEU:HB3	1:G:361:ARG:HA	1.62	0.81
1:D:233:ALA:HB1	1:D:252:LEU:HD11	1.63	0.81
1:C:369:ILE:HG22	1:C:378:HIS:HB2	1.62	0.81
1:H:78:ALA:O	2:H:501:FAD:O3B	1.97	0.81
1:A:259:GLN:NE2	1:A:263:GLU:OE2	2.15	0.80
1:F:180:ARG:NH1	1:F:182:THR:O	2.15	0.79
1:E:133:ALA:HB3	2:E:501:FAD:C5X	2.12	0.79
1:F:328:PRO:CD	2:F:501:FAD:HM71	2.10	0.79
1:G:362:PHE:O	1:G:364:THR:N	2.14	0.79
1:G:160:ARG:NH1	1:G:193:GLY:HA2	1.97	0.79
1:C:79:ALA:HB2	2:C:501:FAD:H51A	1.65	0.78
1:B:9:VAL:HA	1:B:13:GLY:HA3	1.65	0.78
1:F:328:PRO:HB3	2:F:501:FAD:HM72	1.65	0.78
1:D:133:ALA:HB3	2:D:501:FAD:N5	1.97	0.78
1:G:184:LYS:NZ	1:H:153:CYS:SG	2.55	0.77
1:H:133:ALA:O	2:H:501:FAD:C6	2.33	0.77
1:E:75:LEU:HD23	1:E:338:THR:HG21	1.66	0.76
1:G:346:ALA:HB2	1:H:102:VAL:HG21	1.68	0.76
1:H:133:ALA:CB	2:H:501:FAD:N5	2.40	0.76
1:B:96:VAL:HG11	1:B:120:ARG:HG2	1.68	0.76
1:D:24:MET:HE2	1:D:40:PRO:HG2	1.68	0.76
1:D:309:ARG:O	1:D:311:THR:N	2.18	0.75
1:H:133:ALA:HB1	2:H:501:FAD:H6	1.66	0.75
1:C:388:GLU:HB2	1:C:392:ARG:HH12	1.50	0.75
1:A:127:TRP:HB2	1:A:215:LEU:HD12	1.66	0.75
1:D:232:ASP:HA	1:D:235:ARG:HB2	1.69	0.75
1:H:133:ALA:HB3	2:H:501:FAD:C6	2.16	0.75
1:A:232:ASP:O	1:A:234:GLY:N	2.19	0.75
1:C:9:VAL:HA	1:C:13:GLY:HA3	1.67	0.75
1:G:160:ARG:HH22	1:G:193:GLY:HA3	1.52	0.75
1:H:133:ALA:CB	2:H:501:FAD:C6	2.65	0.74
1:E:138:SER:OG	2:E:501:FAD:O5'	2.04	0.74
1:C:415:GLU:CD	2:C:501:FAD:O4	2.31	0.74
1:A:339:GLU:HB3	1:A:379:PRO:HG2	1.70	0.73
1:C:222:THR:HG23	1:C:280:ARG:HE	1.53	0.73
1:G:325:LEU:HA	1:G:328:PRO:HG2	1.70	0.73
1:A:345:LYS:HE2	1:A:374:ASP:HA	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:TYR:CD2	2:D:501:FAD:C7M	2.65	0.73
1:A:331:GLU:OE1	1:A:332:ARG:NH1	2.21	0.73
1:C:339:GLU:HB3	1:C:379:PRO:HG2	1.70	0.73
1:D:20:ASP:HB3	1:D:23:VAL:HG22	1.69	0.73
1:G:283:LEU:O	1:G:285:GLY:N	2.21	0.73
2:C:501:FAD:H2'	2:C:501:FAD:N1	2.02	0.73
1:D:232:ASP:HB3	1:D:235:ARG:CZ	2.19	0.73
1:D:33:GLU:O	1:D:35:ALA:N	2.20	0.72
1:F:205:VAL:HG22	2:F:501:FAD:N1A	2.03	0.72
1:F:328:PRO:CB	2:F:501:FAD:HM72	2.18	0.72
2:G:501:FAD:H2'	2:G:501:FAD:N1	2.03	0.72
1:B:300:GLU:OE1	1:B:300:GLU:N	2.22	0.72
1:E:261:VAL:HG11	1:E:322:ALA:HA	1.69	0.72
1:E:329:ALA:O	1:E:331:GLU:N	2.22	0.72
1:F:328:PRO:CD	2:F:501:FAD:C7M	2.68	0.72
1:G:228:ASP:OD1	1:G:228:ASP:N	2.20	0.72
2:F:501:FAD:O2'	2:F:501:FAD:O4'	2.02	0.72
1:A:252:LEU:HD13	1:A:277:LEU:HD13	1.72	0.72
1:E:143:ASN:OD1	2:E:501:FAD:O4'	2.08	0.71
1:F:134:SER:OG	2:F:501:FAD:O3'	2.08	0.71
1:F:300:GLU:HA	1:F:304:ALA:HB2	1.72	0.71
1:G:267:MET:HB3	1:G:269:LEU:HG	1.72	0.71
1:G:282:ASP:O	1:G:283:LEU:HD23	1.89	0.71
1:G:339:GLU:HB2	1:G:379:PRO:HG2	1.73	0.71
1:B:166:MET:HE1	1:B:195:MET:HG2	1.73	0.71
1:B:362:PHE:O	1:B:364:THR:N	2.24	0.71
1:C:110:PRO:CB	2:C:501:FAD:H62A	1.95	0.71
1:H:328:PRO:CD	2:H:501:FAD:C7M	2.52	0.71
1:B:38:ASP:OD2	1:B:83:ARG:NE	2.23	0.71
1:E:320:PHE:O	1:E:324:ARG:N	2.21	0.70
1:B:339:GLU:HB3	1:B:379:PRO:HG2	1.73	0.70
2:G:501:FAD:O4'	2:G:501:FAD:O2'	2.00	0.70
1:H:328:PRO:HD3	2:H:501:FAD:HM73	1.72	0.70
1:F:371:HIS:HB2	1:F:376:ASN:HB3	1.73	0.70
1:D:38:ASP:OD2	1:D:83:ARG:HG3	1.92	0.69
1:G:283:LEU:HB3	1:G:284:PRO:HD2	1.73	0.69
1:A:290:GLU:O	1:A:294:ARG:HG3	1.91	0.69
1:A:374:ASP:OD2	1:B:184:LYS:NZ	2.25	0.69
1:D:216:ARG:HH22	1:D:282:ASP:CB	2.00	0.69
1:D:216:ARG:NH2	1:D:282:ASP:HB2	2.02	0.69
1:F:34:TRP:CH2	1:F:337:LEU:HB2	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:20:ASP:HB3	1:G:23:VAL:HG22	1.74	0.69
1:A:131:ASP:HB2	1:A:324:ARG:HH22	1.58	0.69
1:G:288:GLY:O	1:G:292:ALA:N	2.24	0.69
1:F:245:ILE:HG22	1:F:246:VAL:H	1.57	0.69
1:B:327:TYR:HB3	2:B:501:FAD:HM72	1.75	0.68
1:B:63:GLY:HA2	1:B:450:ILE:HD11	1.75	0.68
1:E:219:VAL:HG11	1:E:283:LEU:H	1.59	0.68
1:E:106:VAL:HG12	1:E:210:LEU:HB2	1.76	0.68
1:E:133:ALA:CB	2:E:501:FAD:H6	2.23	0.68
1:H:142:GLY:HA3	2:H:501:FAD:O1P	1.92	0.68
1:C:19:THR:HA	1:C:24:MET:HE3	1.76	0.68
1:F:339:GLU:HB3	1:F:379:PRO:HG2	1.76	0.68
1:H:18:VAL:HG21	1:H:45:ARG:HE	1.57	0.68
1:D:237:VAL:HG11	1:D:372:ALA:HB1	1.75	0.68
1:G:160:ARG:HH12	1:G:193:GLY:CA	2.02	0.68
1:D:232:ASP:HA	1:D:235:ARG:CB	2.25	0.67
1:A:327:TYR:HB3	2:A:501:FAD:HM71	1.76	0.67
2:D:501:FAD:H8A	2:D:501:FAD:C5B	2.19	0.67
2:C:501:FAD:O4'	2:C:501:FAD:O2'	2.02	0.67
1:D:329:ALA:O	1:D:331:GLU:N	2.27	0.67
1:D:266:ASN:OD1	1:D:266:ASN:N	2.27	0.66
1:D:327:TYR:HB3	2:D:501:FAD:HM71	1.76	0.66
1:E:76:SER:OG	1:E:418:VAL:O	2.13	0.66
1:C:224:VAL:HG12	1:C:225:GLY:H	1.61	0.66
1:B:226:TYR:CZ	1:B:276:LEU:HD13	2.31	0.66
1:G:399:GLU:HG3	1:G:424:ARG:HH22	1.61	0.66
1:B:297:GLU:HB3	1:B:301:LYS:HE3	1.77	0.66
1:D:7:GLU:OE1	1:D:62:ARG:NH1	2.29	0.65
1:A:44:VAL:HG11	1:A:55:VAL:HG11	1.77	0.65
1:C:224:VAL:HG13	1:C:307:ALA:HA	1.78	0.65
1:C:224:VAL:HG21	1:C:299:PHE:HD2	1.60	0.65
1:A:133:ALA:HB3	2:A:501:FAD:N5	2.12	0.65
1:E:316:ALA:HA	1:E:319:LEU:HD13	1.78	0.65
1:D:16:GLN:OE1	1:D:92:ARG:NH1	2.26	0.65
1:H:413:THR:HB	1:H:422:LYS:HZ3	1.61	0.65
1:A:347:ARG:HH21	1:G:350:HIS:CE1	2.14	0.65
1:F:138:SER:OG	2:F:501:FAD:H4'	1.97	0.65
1:H:134:SER:HG	2:H:501:FAD:C9A	2.06	0.65
1:D:230:LEU:HA	1:D:275:VAL:HG11	1.78	0.65
1:C:134:SER:OG	2:C:501:FAD:H1'2	1.97	0.65
1:E:133:ALA:HB1	2:E:501:FAD:H6	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:ALA:HA	1:C:319:LEU:HD13	1.78	0.64
1:D:156:TYR:OH	1:D:216:ARG:NH1	2.29	0.64
1:G:340:ASP:HB2	1:G:416:HIS:HD2	1.61	0.64
2:A:501:FAD:N1	2:A:501:FAD:H2'	2.12	0.64
1:B:167:GLU:HB3	1:B:207:GLU:HB3	1.79	0.64
1:A:289:GLN:NE2	1:A:290:GLU:HG3	2.12	0.64
1:B:76:SER:OG	1:B:418:VAL:O	2.16	0.64
1:F:216:ARG:HH21	1:F:282:ASP:HB3	1.63	0.64
1:G:134:SER:OG	2:G:501:FAD:O3'	2.15	0.64
1:A:170:VAL:HG22	1:A:171:GLY:H	1.63	0.64
1:A:378:HIS:NE2	1:A:415:GLU:OE2	2.30	0.64
1:E:73:THR:O	2:E:501:FAD:HM81	1.97	0.64
1:G:249:ALA:HB3	1:G:280:ARG:HG3	1.79	0.64
1:H:73:THR:O	2:H:501:FAD:O3'	2.15	0.64
1:F:327:TYR:H	1:F:328:PRO:HD2	1.63	0.64
1:C:108:VAL:HG11	1:C:117:LEU:HD12	1.79	0.64
1:G:327:TYR:HB3	2:G:501:FAD:HM71	1.80	0.63
1:G:258:LEU:HD11	1:G:276:LEU:HD13	1.81	0.63
1:A:388:GLU:HG2	1:A:389:GLU:N	2.11	0.63
1:C:278:LEU:HD11	1:C:319:LEU:HB3	1.80	0.63
1:C:313:GLU:O	1:C:316:ALA:N	2.31	0.63
1:D:9:VAL:HA	1:D:13:GLY:HA3	1.79	0.63
1:D:53:ALA:HA	1:D:169:VAL:HG11	1.80	0.63
1:F:255:ARG:NH2	1:F:270:SER:O	2.32	0.63
1:E:226:TYR:HB3	1:E:276:LEU:HA	1.80	0.63
1:H:4:VAL:HG22	1:H:62:ARG:HD2	1.81	0.63
1:D:231:THR:OG1	1:D:235:ARG:NH1	2.32	0.63
1:G:296:LEU:HG	1:G:309:ARG:HD2	1.81	0.63
1:G:170:VAL:HG12	1:G:171:GLY:H	1.63	0.62
1:H:351:MET:HE1	1:H:404:GLU:HG3	1.81	0.62
1:F:113:VAL:HG22	1:F:116:ASP:H	1.64	0.62
1:D:293:ASP:OD1	1:D:294:ARG:N	2.30	0.62
1:A:133:ALA:HA	1:A:324:ARG:HH11	1.64	0.62
2:F:501:FAD:N1	2:F:501:FAD:H2'	2.12	0.62
1:E:133:ALA:HB3	2:E:501:FAD:C6	2.29	0.62
1:E:264:TRP:CZ2	1:G:25:GLU:HB3	2.34	0.62
1:D:106:VAL:HG22	1:D:212:LEU:HD21	1.80	0.62
1:C:144:VAL:HG13	1:C:196:VAL:HG22	1.80	0.62
1:E:219:VAL:HG22	1:E:285:GLY:H	1.65	0.62
1:D:378:HIS:CE1	1:D:415:GLU:OE2	2.52	0.62
1:E:133:ALA:CB	2:E:501:FAD:N5	2.40	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:228:ASP:HB3	1:G:274:GLU:N	2.11	0.62
1:B:118:ARG:NH2	1:B:130:PRO:O	2.33	0.62
1:F:118:ARG:NH2	1:F:135:SER:OG	2.33	0.61
1:B:310:SER:OG	1:B:312:ASP:OD1	2.17	0.61
1:C:75:LEU:HD11	2:C:501:FAD:C7M	2.30	0.61
1:F:138:SER:HB2	2:F:501:FAD:O3'	1.99	0.61
1:A:286:THR:O	1:A:289:GLN:HG3	2.00	0.61
1:E:75:LEU:CD1	2:E:501:FAD:C9	2.79	0.61
1:F:345:LYS:HE2	1:F:374:ASP:HA	1.81	0.61
1:F:459:LEU:O	1:F:460:GLU:HG2	2.00	0.61
1:H:328:PRO:CD	2:H:501:FAD:HM71	2.22	0.61
1:A:228:ASP:OD1	1:A:228:ASP:N	2.33	0.61
1:A:253:ILE:HG13	1:A:369:ILE:HG22	1.83	0.61
1:D:4:VAL:HG13	1:D:62:ARG:HH21	1.64	0.61
1:F:342:CYS:HB3	1:F:411:THR:HG22	1.83	0.61
1:D:291:GLU:O	1:D:295:ILE:N	2.30	0.61
1:D:355:ILE:HG22	1:D:366:ILE:HG21	1.81	0.61
1:A:227:PHE:O	1:A:274:GLU:N	2.25	0.60
1:E:254:ASP:HA	1:E:275:VAL:HA	1.83	0.60
1:A:184:LYS:NZ	1:B:374:ASP:OD2	2.26	0.60
1:B:308:VAL:C	1:B:310:SER:H	2.10	0.60
1:C:255:ARG:HB2	1:C:274:GLU:HA	1.82	0.60
1:G:133:ALA:H	2:G:501:FAD:C4	2.14	0.60
1:B:329:ALA:C	1:B:331:GLU:H	2.10	0.60
1:G:79:ALA:HB2	2:G:501:FAD:H3B	1.83	0.60
1:G:133:ALA:HA	1:G:324:ARG:NH1	2.17	0.60
1:A:205:VAL:O	2:A:501:FAD:N6A	2.35	0.60
1:B:327:TYR:HE1	1:B:336:LEU:HD22	1.66	0.60
1:G:106:VAL:HG22	1:G:212:LEU:HD21	1.83	0.60
2:H:501:FAD:H8A	2:H:501:FAD:O5B	2.02	0.60
1:D:255:ARG:HB2	1:D:274:GLU:HA	1.83	0.59
1:F:255:ARG:NH2	1:F:259:GLN:OE1	2.35	0.59
1:E:20:ASP:HB3	1:E:23:VAL:HG12	1.82	0.59
1:C:313:GLU:O	1:C:317:GLU:N	2.25	0.59
1:D:248:SER:HB2	1:D:282:ASP:CG	2.27	0.59
1:F:337:LEU:HD23	1:F:398:PHE:HD2	1.66	0.59
1:F:355:ILE:HD13	1:F:401:ILE:HD12	1.83	0.59
1:A:23:VAL:HG23	1:F:23:VAL:HG13	1.85	0.59
1:A:360:GLU:O	1:H:95:ARG:NH1	2.35	0.59
1:C:280:ARG:NH2	1:C:313:GLU:OE2	2.36	0.59
1:E:134:SER:CB	2:E:501:FAD:HO3'	2.09	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:333:LEU:HD23	1:G:385:ALA:HB1	1.83	0.59
1:F:34:TRP:HB2	1:F:421:LEU:HD22	1.84	0.59
1:D:388:GLU:O	1:D:391:LYS:HB3	2.02	0.59
1:D:264:TRP:HZ3	1:D:332:ARG:HD2	1.67	0.59
1:G:132:PRO:C	1:G:324:ARG:HH12	2.10	0.59
1:H:79:ALA:HB2	2:H:501:FAD:H3B	1.85	0.59
1:A:73:THR:OG1	2:A:501:FAD:O3'	2.08	0.58
1:D:363:ASP:HB3	1:D:393:ARG:NH2	2.18	0.58
1:E:339:GLU:HB2	1:E:379:PRO:HG2	1.85	0.58
1:A:388:GLU:HB2	1:F:388:GLU:OE2	2.04	0.58
1:F:15:GLU:OE2	1:F:92:ARG:NH2	2.37	0.58
1:C:44:VAL:HG11	1:C:55:VAL:HG21	1.85	0.58
1:C:289:GLN:HE21	1:C:293:ASP:HB2	1.67	0.58
1:E:223:VAL:HG21	1:E:295:ILE:HG13	1.83	0.58
1:D:325:LEU:HA	1:D:328:PRO:HG2	1.84	0.58
1:C:75:LEU:HD11	2:C:501:FAD:C7	2.33	0.58
1:G:391:LYS:HZ3	1:G:395:LYS:HD2	1.67	0.58
1:F:392:ARG:HA	1:F:395:LYS:HB3	1.86	0.58
1:G:134:SER:HG	2:G:501:FAD:HO3'	1.46	0.58
1:D:293:ASP:O	1:D:296:LEU:HB2	2.03	0.58
1:E:340:ASP:HB2	1:E:416:HIS:HD2	1.68	0.58
1:B:290:GLU:O	1:B:292:ALA:N	2.36	0.58
1:E:343:VAL:HG21	1:E:351:MET:HG3	1.84	0.58
2:E:501:FAD:H2'	2:E:501:FAD:N1	2.13	0.58
1:F:340:ASP:O	1:F:413:THR:HA	2.04	0.57
1:E:415:GLU:HB2	2:E:501:FAD:O2	2.03	0.57
1:B:234:GLY:HA3	1:B:349:PRO:HB3	1.86	0.57
1:C:222:THR:HG23	1:C:280:ARG:NE	2.19	0.57
1:F:311:THR:OG1	1:F:312:ASP:N	2.32	0.57
1:G:158:VAL:HG22	1:G:159:THR:H	1.69	0.57
1:G:374:ASP:HB2	1:H:183:ALA:HB3	1.87	0.57
1:C:149:GLY:H	2:C:501:FAD:HN3	1.52	0.57
1:E:41:ALA:HB2	1:E:84:GLY:HA2	1.85	0.57
1:E:219:VAL:HG11	1:E:283:LEU:N	2.18	0.57
1:F:337:LEU:HD23	1:F:398:PHE:CD2	2.39	0.57
1:C:132:PRO:O	1:C:134:SER:N	2.34	0.57
1:D:8:LEU:HB3	1:D:17:VAL:HG21	1.86	0.57
1:D:298:CYS:HA	1:D:301:LYS:HE2	1.87	0.57
1:H:24:MET:HG3	1:H:43:VAL:HG23	1.87	0.57
1:A:198:SER:O	1:A:201:THR:HG22	2.04	0.57
1:B:27:TYR:CD2	1:B:43:VAL:HG11	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:PRO:C	1:C:134:SER:H	2.12	0.57
1:A:22:ALA:O	1:F:26:GLY:HA3	2.04	0.57
1:G:265:LYS:HD2	1:G:325:LEU:HD21	1.86	0.57
1:D:41:ALA:HB2	1:D:84:GLY:HA2	1.86	0.56
1:G:53:ALA:HA	1:G:169:VAL:HG11	1.86	0.56
1:G:239:ALA:HA	1:G:242:ALA:HB3	1.87	0.56
1:E:226:TYR:CB	1:E:276:LEU:HA	2.35	0.56
1:F:247:PRO:O	1:F:249:ALA:N	2.36	0.56
1:D:114:ASN:OD1	1:D:132:PRO:HD2	2.04	0.56
1:D:76:SER:O	1:D:420:LEU:N	2.30	0.56
1:G:155:LYS:NZ	1:G:283:LEU:HD21	2.21	0.56
1:G:227:PHE:O	1:G:229:SER:N	2.38	0.56
1:D:43:VAL:HG22	1:D:87:VAL:HB	1.88	0.56
1:F:452:ASN:HD21	1:F:455:LYS:HD2	1.71	0.56
1:G:120:ARG:NH1	1:G:124:ASP:OD1	2.37	0.56
1:H:96:VAL:HG13	1:H:108:VAL:HG12	1.88	0.56
1:F:351:MET:HG3	1:F:377:LEU:HD11	1.86	0.56
1:G:223:VAL:HG13	1:G:309:ARG:HA	1.87	0.56
1:H:78:ALA:O	1:H:455:LYS:NZ	2.34	0.56
1:C:297:GLU:HA	1:C:300:GLU:OE2	2.06	0.56
1:E:289:GLN:HA	1:E:292:ALA:HB3	1.87	0.56
1:F:34:TRP:HH2	1:F:337:LEU:HB2	1.71	0.56
1:G:444:ALA:HB1	1:H:440:ALA:HB1	1.88	0.56
1:D:363:ASP:HB3	1:D:393:ARG:HH21	1.71	0.56
1:F:236:ALA:HA	1:F:239:ALA:HB3	1.88	0.56
1:F:223:VAL:HA	1:F:309:ARG:HA	1.89	0.55
1:F:325:LEU:O	1:F:330:LEU:HD13	2.06	0.55
1:F:351:MET:HG3	1:F:377:LEU:CD1	2.36	0.55
1:G:445:LEU:HD11	1:H:441:VAL:HG22	1.87	0.55
1:B:265:LYS:O	1:B:267:MET:N	2.39	0.55
1:F:12:ILE:O	1:F:16:GLN:HB2	2.06	0.55
1:F:367:GLY:N	1:F:380:LEU:O	2.39	0.55
1:B:398:PHE:O	1:B:402:VAL:HG23	2.07	0.55
1:G:276:LEU:CD2	1:G:278:LEU:HD13	2.36	0.55
1:A:234:GLY:O	1:A:237:VAL:N	2.35	0.55
2:B:501:FAD:H2'	2:B:501:FAD:N1	2.19	0.55
1:D:38:ASP:OD1	1:D:39:ALA:N	2.39	0.55
1:A:99:VAL:HG22	1:A:106:VAL:HG23	1.89	0.55
1:A:237:VAL:HG11	1:A:372:ALA:HB1	1.87	0.55
1:D:44:VAL:HG11	1:D:55:VAL:HG11	1.88	0.55
2:G:501:FAD:N1	2:G:501:FAD:C2'	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:VAL:HG12	1:B:385:ALA:H	1.70	0.55
1:E:24:MET:HE2	1:E:40:PRO:HG2	1.89	0.55
1:H:149:GLY:H	1:H:415:GLU:HB2	1.70	0.55
1:A:290:GLU:HA	1:A:293:ASP:OD1	2.07	0.55
1:C:106:VAL:HG13	1:C:212:LEU:HD11	1.88	0.55
1:C:224:VAL:HG22	1:C:296:LEU:HD13	1.89	0.55
1:E:108:VAL:HG11	1:E:117:LEU:HD13	1.89	0.55
1:C:198:SER:O	1:C:201:THR:HG22	2.07	0.55
1:E:245:ILE:HD12	1:E:291:GLU:OE1	2.06	0.54
1:G:75:LEU:HD12	1:G:416:HIS:CE1	2.42	0.54
1:A:164:LEU:HD11	1:A:211:ARG:HB3	1.89	0.54
1:B:264:TRP:CG	1:B:332:ARG:HH12	2.25	0.54
1:F:247:PRO:C	1:F:249:ALA:H	2.15	0.54
1:C:281:SER:CB	1:C:292:ALA:HB2	2.36	0.54
1:D:320:PHE:O	1:D:324:ARG:N	2.31	0.54
1:F:397:ALA:O	1:F:401:ILE:HG12	2.08	0.54
1:H:167:GLU:HB3	1:H:207:GLU:HB3	1.88	0.54
1:B:251:GLU:O	1:B:277:LEU:HA	2.07	0.54
2:B:501:FAD:N1	2:B:501:FAD:C2'	2.71	0.54
1:C:132:PRO:HB3	1:C:148:ALA:HB1	1.90	0.54
1:B:327:TYR:CD2	2:B:501:FAD:HM72	2.43	0.54
1:C:362:PHE:HB3	1:C:393:ARG:HB3	1.89	0.54
1:D:233:ALA:HB1	1:D:252:LEU:CD1	2.35	0.54
2:F:501:FAD:N1	2:F:501:FAD:C2'	2.69	0.54
1:G:43:VAL:HG22	1:G:87:VAL:HB	1.90	0.54
1:G:108:VAL:HG11	1:G:117:LEU:HD12	1.88	0.54
1:G:237:VAL:HG11	1:G:372:ALA:HB1	1.90	0.54
1:H:75:LEU:HD23	2:H:501:FAD:H1'1	1.89	0.54
1:B:221:HIS:CD2	1:B:292:ALA:HB1	2.42	0.54
1:D:232:ASP:HB3	1:D:235:ARG:NE	2.22	0.54
2:D:501:FAD:C2'	2:D:501:FAD:N1	2.71	0.54
1:B:221:HIS:HE1	1:B:295:ILE:HD11	1.72	0.53
1:C:96:VAL:HG13	1:C:108:VAL:HG12	1.90	0.53
1:D:231:THR:O	1:D:235:ARG:HG3	2.08	0.53
1:F:224:VAL:HG21	1:F:277:LEU:HB3	1.90	0.53
1:H:235:ARG:HG3	1:H:238:ALA:HB3	1.89	0.53
2:A:501:FAD:N1	2:A:501:FAD:C2'	2.71	0.53
1:C:3:GLY:O	1:C:5:VAL:N	2.40	0.53
1:C:158:VAL:HG22	1:C:159:THR:H	1.73	0.53
1:D:321:GLN:HA	1:D:324:ARG:HB2	1.90	0.53
1:E:75:LEU:HD11	2:E:501:FAD:C8	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:269:LEU:O	1:F:271:ALA:N	2.42	0.53
1:H:158:VAL:HG22	1:H:159:THR:H	1.72	0.53
1:A:290:GLU:O	1:A:294:ARG:N	2.42	0.53
1:D:294:ARG:HA	1:D:297:GLU:HG2	1.89	0.53
1:B:264:TRP:HZ3	1:B:325:LEU:HD23	1.73	0.53
1:D:105:THR:HA	1:D:212:LEU:HD23	1.90	0.53
1:C:415:GLU:HB2	2:C:501:FAD:N3	2.23	0.53
1:E:75:LEU:HD11	2:E:501:FAD:C9	2.38	0.53
1:E:351:MET:O	1:E:355:ILE:HG12	2.08	0.53
1:F:363:ASP:HB3	1:F:393:ARG:NH2	2.14	0.53
1:G:135:SER:OG	1:G:136:PRO:HD3	2.09	0.53
1:G:310:SER:OG	1:G:312:ASP:OD1	2.23	0.53
1:A:308:VAL:HG13	1:A:310:SER:HB2	1.89	0.53
1:D:73:THR:OG1	2:D:501:FAD:O2P	2.22	0.53
1:D:227:PHE:HB3	1:D:232:ASP:OD2	2.08	0.53
1:F:340:ASP:OD2	1:F:414:GLY:N	2.37	0.53
1:H:158:VAL:HG13	1:H:160:ARG:H	1.74	0.53
1:C:351:MET:O	1:C:355:ILE:HG12	2.08	0.53
1:F:232:ASP:OD1	1:F:233:ALA:N	2.42	0.53
1:F:257:CYS:O	1:F:261:VAL:HG23	2.08	0.53
1:H:112:VAL:HG13	1:H:140:ILE:HD13	1.91	0.53
1:B:198:SER:O	1:B:201:THR:HG22	2.09	0.53
1:B:221:HIS:HA	1:B:311:THR:HG23	1.91	0.53
1:C:388:GLU:HB2	1:C:392:ARG:NH1	2.22	0.53
1:E:198:SER:O	1:E:201:THR:HG22	2.09	0.52
1:C:15:GLU:HG2	1:C:16:GLN:OE1	2.08	0.52
1:D:228:ASP:HB2	1:D:303:LYS:NZ	2.23	0.52
1:G:27:TYR:CD2	1:G:43:VAL:HG11	2.45	0.52
1:H:106:VAL:HG22	1:H:212:LEU:HD11	1.90	0.52
1:A:289:GLN:HE22	1:A:290:GLU:HG3	1.72	0.52
1:D:158:VAL:HG22	1:D:159:THR:H	1.72	0.52
1:H:133:ALA:O	2:H:501:FAD:C7	2.58	0.52
1:H:371:HIS:HB2	1:H:376:ASN:HB3	1.91	0.52
1:B:106:VAL:HG21	1:B:117:LEU:HD11	1.90	0.52
2:B:501:FAD:O4'	2:B:501:FAD:O2'	2.11	0.52
1:C:330:LEU:HB3	1:C:336:LEU:HD22	1.92	0.52
1:E:252:LEU:O	1:E:369:ILE:HA	2.10	0.52
1:F:255:ARG:CZ	1:F:259:GLN:HB2	2.38	0.52
2:H:501:FAD:N1	2:H:501:FAD:C2'	2.72	0.52
1:B:297:GLU:HA	1:B:300:GLU:CD	2.34	0.52
1:B:308:VAL:O	1:B:310:SER:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:12:ILE:HD12	1:F:16:GLN:HG2	1.91	0.52
1:F:224:VAL:HB	1:F:278:LEU:H	1.75	0.52
1:G:399:GLU:HG3	1:G:424:ARG:NH2	2.23	0.52
1:C:224:VAL:HG21	1:C:299:PHE:CD2	2.42	0.52
1:D:33:GLU:C	1:D:35:ALA:H	2.15	0.52
1:C:8:LEU:HD12	1:C:58:ILE:HG21	1.92	0.52
1:C:219:VAL:HG11	1:C:283:LEU:O	2.09	0.52
1:A:230:LEU:HB3	1:A:352:LEU:HB3	1.91	0.52
1:A:234:GLY:O	1:A:236:ALA:N	2.43	0.52
1:B:221:HIS:CE1	1:B:295:ILE:HD11	2.45	0.52
1:B:395:LYS:O	1:B:399:GLU:HG3	2.09	0.52
1:C:282:ASP:C	1:C:283:LEU:HD12	2.35	0.52
1:C:343:VAL:HG11	1:C:351:MET:SD	2.50	0.52
2:E:501:FAD:N1	2:E:501:FAD:C2'	2.71	0.52
1:G:4:VAL:O	1:G:6:GLU:N	2.34	0.52
1:D:106:VAL:HG11	1:D:121:VAL:HG12	1.92	0.52
1:B:329:ALA:O	1:B:330:LEU:HB2	2.10	0.52
1:H:354:ALA:O	1:H:358:ALA:N	2.43	0.52
1:A:278:LEU:HD11	1:A:319:LEU:HB3	1.92	0.51
1:G:105:THR:HA	1:G:212:LEU:HD23	1.93	0.51
1:H:133:ALA:CB	2:H:501:FAD:C5X	2.84	0.51
1:H:108:VAL:HG11	1:H:117:LEU:HD12	1.92	0.51
1:B:90:PHE:HZ	1:B:204:LEU:HB3	1.76	0.51
1:C:253:ILE:HG22	1:C:276:LEU:HB3	1.91	0.51
1:D:228:ASP:HB2	1:D:303:LYS:HZ1	1.75	0.51
1:E:133:ALA:CB	2:E:501:FAD:C6	2.88	0.51
1:F:127:TRP:N	1:F:213:VAL:O	2.43	0.51
1:F:452:ASN:ND2	1:F:455:LYS:HD2	2.26	0.51
1:D:231:THR:O	1:D:235:ARG:N	2.35	0.51
1:D:253:ILE:HG13	1:D:369:ILE:HG22	1.92	0.51
1:G:178:LEU:HD21	1:H:437:MET:HE1	1.93	0.51
1:C:318:ALA:HA	1:C:321:GLN:OE1	2.11	0.51
1:D:119:ALA:O	1:D:123:GLN:HG3	2.11	0.51
1:F:3:GLY:O	1:F:5:VAL:N	2.43	0.51
1:G:282:ASP:C	1:G:283:LEU:HD23	2.35	0.51
1:A:247:PRO:HB3	1:A:295:ILE:HD13	1.92	0.51
1:A:340:ASP:O	1:A:413:THR:HA	2.11	0.51
1:C:287:SER:O	1:C:290:GLU:HG2	2.11	0.51
1:D:234:GLY:HA3	1:D:349:PRO:HA	1.92	0.51
1:G:278:LEU:HB3	1:G:320:PHE:CZ	2.46	0.51
1:A:68:GLY:O	2:A:501:FAD:H2B	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:SER:OG	2:C:501:FAD:C1'	2.59	0.51
1:E:73:THR:HB	2:E:501:FAD:HM81	1.92	0.51
1:B:277:LEU:HD22	1:B:299:PHE:HZ	1.76	0.51
1:C:90:PHE:HZ	1:C:204:LEU:HB3	1.76	0.51
1:C:439:ARG:HG2	1:C:459:LEU:HD13	1.92	0.51
1:E:249:ALA:HB3	1:E:280:ARG:HB2	1.93	0.51
1:F:34:TRP:CZ3	1:F:337:LEU:HD13	2.46	0.51
1:G:437:MET:HE1	1:H:178:LEU:HD21	1.92	0.51
1:B:352:LEU:HD23	1:B:355:ILE:HD11	1.92	0.51
1:D:226:TYR:O	1:D:227:PHE:HB2	2.10	0.51
1:E:20:ASP:O	1:E:24:MET:HB3	2.10	0.51
1:A:52:VAL:HG23	1:A:93:MET:HE1	1.92	0.50
1:B:144:VAL:HG13	1:B:196:VAL:HG22	1.92	0.50
1:C:38:ASP:OD1	1:C:39:ALA:N	2.38	0.50
1:G:293:ASP:C	1:G:295:ILE:H	2.19	0.50
1:C:326:ALA:O	1:C:330:LEU:HD13	2.10	0.50
1:C:415:GLU:CG	2:C:501:FAD:O4	2.59	0.50
1:D:230:LEU:HD23	1:D:356:GLU:HB2	1.92	0.50
1:D:312:ASP:O	1:D:314:GLU:N	2.32	0.50
1:E:135:SER:OG	1:E:136:PRO:HD3	2.11	0.50
1:E:142:GLY:HA2	2:E:501:FAD:C8A	2.40	0.50
1:E:376:ASN:ND2	1:E:414:GLY:HA3	2.25	0.50
1:F:337:LEU:HD12	1:F:338:THR:N	2.26	0.50
1:E:138:SER:HG	2:E:501:FAD:P	2.34	0.50
1:G:134:SER:HG	1:G:138:SER:HB3	1.76	0.50
1:D:278:LEU:HD11	1:D:319:LEU:HB3	1.94	0.50
1:F:371:HIS:N	1:F:376:ASN:O	2.45	0.50
1:G:223:VAL:HG22	1:G:309:ARG:HG3	1.94	0.50
1:A:46:PRO:HB2	1:A:93:MET:HE3	1.94	0.50
1:C:16:GLN:OE1	1:C:92:ARG:NH1	2.44	0.50
2:D:501:FAD:N1	2:D:501:FAD:O2'	2.40	0.50
1:E:283:LEU:HD11	1:E:291:GLU:OE1	2.10	0.50
1:H:341:VAL:HG23	1:H:377:LEU:HD12	1.94	0.50
1:B:226:TYR:CD2	1:B:272:GLU:HA	2.47	0.50
1:D:282:ASP:C	1:D:283:LEU:HD12	2.37	0.50
1:A:178:LEU:HD21	1:B:437:MET:HE1	1.94	0.50
1:A:283:LEU:HB2	1:A:288:GLY:CA	2.42	0.50
1:B:276:LEU:HD21	1:B:319:LEU:HD23	1.94	0.50
1:D:347:ARG:HG2	1:D:408:VAL:HG13	1.94	0.50
1:E:365:ARG:O	1:E:365:ARG:HG3	2.11	0.50
1:F:278:LEU:HD22	1:F:320:PHE:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:VAL:HA	1:A:278:LEU:HD23	1.94	0.50
1:A:283:LEU:HB2	1:A:288:GLY:HA2	1.92	0.50
1:C:284:PRO:O	1:C:287:SER:HB2	2.12	0.50
1:G:160:ARG:HH22	1:G:193:GLY:CA	2.21	0.50
1:G:229:SER:C	1:G:231:THR:H	2.20	0.50
1:C:24:MET:HE2	1:C:43:VAL:HG23	1.94	0.49
1:E:134:SER:CB	2:E:501:FAD:O3'	2.59	0.49
1:A:23:VAL:CG2	1:F:23:VAL:HG13	2.41	0.49
1:C:330:LEU:HG	1:C:333:LEU:HD12	1.94	0.49
1:D:294:ARG:O	1:D:297:GLU:HB2	2.12	0.49
1:B:257:CYS:O	1:B:261:VAL:HG23	2.12	0.49
1:F:150:GLY:N	1:F:153:CYS:SG	2.74	0.49
1:A:59:CYS:HA	1:A:64:VAL:HG12	1.93	0.49
1:E:27:TYR:HD2	1:E:43:VAL:HG11	1.77	0.49
1:E:138:SER:OG	2:E:501:FAD:C5'	2.60	0.49
1:E:340:ASP:O	1:E:413:THR:HA	2.13	0.49
1:F:278:LEU:HB3	1:F:320:PHE:CZ	2.48	0.49
1:A:300:GLU:C	1:A:302:GLU:H	2.21	0.49
1:C:347:ARG:HG3	1:C:408:VAL:HG13	1.95	0.49
1:D:127:TRP:HB2	1:D:215:LEU:HD13	1.94	0.49
1:A:167:GLU:HB3	1:A:207:GLU:HB3	1.95	0.49
1:C:69:ARG:NH2	1:C:72:GLY:HA3	2.27	0.49
1:A:205:VAL:HG11	1:A:208:VAL:HG23	1.95	0.49
1:G:289:GLN:CD	1:G:309:ARG:HH22	2.20	0.49
1:G:355:ILE:HD11	1:G:379:PRO:HB3	1.94	0.49
1:C:281:SER:HB2	1:C:292:ALA:HB2	1.95	0.49
1:H:114:ASN:HB3	1:H:135:SER:HA	1.94	0.49
1:A:52:VAL:HA	1:A:55:VAL:HG22	1.94	0.49
1:D:224:VAL:HG21	1:D:308:VAL:H	1.77	0.49
1:D:296:LEU:O	1:D:299:PHE:N	2.44	0.49
1:A:162:TYR:O	1:A:210:LEU:HA	2.12	0.48
1:C:99:VAL:HG22	1:C:106:VAL:HG12	1.94	0.48
1:A:115:ASP:OD1	1:A:118:ARG:NH1	2.46	0.48
1:E:118:ARG:NH2	1:E:130:PRO:O	2.44	0.48
1:E:255:ARG:N	1:E:274:GLU:O	2.44	0.48
1:F:331:GLU:O	1:F:333:LEU:N	2.45	0.48
1:G:134:SER:OG	1:G:138:SER:HB3	2.13	0.48
1:G:276:LEU:HD21	1:G:278:LEU:HD13	1.93	0.48
1:H:29:HIS:HB3	1:H:37:TYR:CG	2.47	0.48
1:C:106:VAL:HG23	1:C:210:LEU:HB2	1.94	0.48
1:G:182:THR:HG22	1:G:183:ALA:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:340:ASP:O	1:G:413:THR:HA	2.14	0.48
1:E:294:ARG:HA	1:E:297:GLU:HG2	1.94	0.48
1:F:281:SER:OG	1:F:291:GLU:HB2	2.13	0.48
1:F:355:ILE:O	1:F:359:GLY:N	2.46	0.48
1:G:296:LEU:O	1:G:300:GLU:N	2.43	0.48
1:C:351:MET:HE3	1:C:351:MET:HB2	1.62	0.48
1:D:327:TYR:CE2	2:D:501:FAD:HM82	2.48	0.48
1:H:27:TYR:OH	1:H:45:ARG:NH1	2.46	0.48
1:B:290:GLU:C	1:B:292:ALA:H	2.22	0.48
1:B:371:HIS:N	1:B:376:ASN:O	2.47	0.48
1:C:415:GLU:HB2	2:C:501:FAD:HN3	1.79	0.48
1:E:264:TRP:HZ3	1:G:37:TYR:CE2	2.31	0.48
1:E:290:GLU:HG3	1:E:291:GLU:HG3	1.96	0.48
1:H:133:ALA:HB3	2:H:501:FAD:H6	1.80	0.48
1:H:144:VAL:HG13	1:H:196:VAL:HG22	1.94	0.48
1:A:250:LEU:HD13	1:A:279:ALA:HB2	1.95	0.48
1:F:144:VAL:HG13	1:F:196:VAL:HG22	1.95	0.48
1:A:251:GLU:O	1:A:277:LEU:HD12	2.14	0.48
1:C:236:ALA:N	1:C:302:GLU:OE2	2.47	0.48
1:F:96:VAL:HG22	1:F:108:VAL:HG12	1.96	0.48
1:G:106:VAL:HG11	1:G:121:VAL:HG12	1.96	0.48
1:E:282:ASP:C	1:E:283:LEU:HD23	2.39	0.48
1:E:317:GLU:OE1	1:E:317:GLU:N	2.38	0.48
1:E:376:ASN:HD21	1:E:414:GLY:HA3	1.79	0.48
1:F:151:LEU:HG	1:F:371:HIS:HE1	1.79	0.48
1:C:344:PRO:HD2	1:C:408:VAL:HG12	1.95	0.48
1:D:227:PHE:CE1	1:D:304:ALA:HA	2.48	0.48
1:D:232:ASP:O	1:D:236:ALA:N	2.47	0.47
1:E:127:TRP:CH2	1:E:216:ARG:HD2	2.49	0.47
1:E:315:GLU:HG2	1:E:318:ALA:HB3	1.96	0.47
1:G:302:GLU:O	1:G:304:ALA:N	2.47	0.47
1:G:383:VAL:HG12	1:G:385:ALA:H	1.79	0.47
1:G:169:VAL:HG22	1:G:175:VAL:HG12	1.96	0.47
1:D:118:ARG:HA	1:D:121:VAL:HG22	1.97	0.47
1:F:328:PRO:CD	2:F:501:FAD:HM72	2.44	0.47
1:C:399:GLU:HG2	1:C:424:ARG:HH22	1.78	0.47
1:E:233:ALA:O	1:E:237:VAL:HB	2.15	0.47
1:H:3:GLY:O	1:H:5:VAL:N	2.41	0.47
1:H:31:GLU:OE1	1:H:73:THR:HA	2.14	0.47
1:C:412:VAL:HG21	1:C:426:ALA:HB2	1.97	0.47
1:D:232:ASP:HB3	1:D:235:ARG:NH2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:PHE:CZ	1:E:277:LEU:HD22	2.50	0.47
1:E:313:GLU:OE2	1:E:315:GLU:HB3	2.15	0.47
2:C:501:FAD:N1	2:C:501:FAD:C2'	2.72	0.47
1:D:9:VAL:HA	1:D:13:GLY:CA	2.45	0.47
1:F:73:THR:OG1	2:F:501:FAD:H3'	2.14	0.47
1:F:378:HIS:NE2	1:F:415:GLU:OE2	2.44	0.47
1:G:232:ASP:OD1	1:G:233:ALA:N	2.48	0.47
1:B:340:ASP:O	1:B:413:THR:HA	2.14	0.47
1:E:134:SER:OG	2:E:501:FAD:O3'	1.76	0.47
1:E:253:ILE:O	1:E:276:LEU:N	2.36	0.47
1:E:253:ILE:HA	1:E:369:ILE:HG22	1.97	0.47
1:E:335:PRO:HD3	1:G:333:LEU:HA	1.96	0.47
1:G:278:LEU:HD23	1:G:320:PHE:CZ	2.50	0.47
1:H:413:THR:HB	1:H:422:LYS:NZ	2.29	0.47
1:D:351:MET:O	1:D:355:ILE:HG12	2.15	0.47
1:F:38:ASP:OD1	1:F:39:ALA:N	2.42	0.47
1:F:220:GLU:HG3	1:F:280:ARG:HE	1.79	0.47
1:H:398:PHE:HD1	1:H:401:ILE:HD12	1.80	0.47
1:A:19:THR:HA	1:A:24:MET:HE3	1.97	0.47
1:A:25:GLU:OE2	1:F:29:HIS:NE2	2.47	0.47
1:C:223:VAL:HG13	1:C:224:VAL:HG23	1.96	0.47
1:F:32:ALA:HB1	1:F:421:LEU:HD11	1.97	0.47
1:G:99:VAL:HG13	1:G:106:VAL:HG12	1.97	0.47
1:C:114:ASN:OD1	1:C:132:PRO:HD2	2.15	0.46
1:C:365:ARG:NH1	1:C:382:ILE:HG22	2.30	0.46
1:E:72:GLY:N	2:E:501:FAD:O2A	2.46	0.46
1:F:355:ILE:HA	1:F:401:ILE:HD11	1.96	0.46
1:B:343:VAL:HG21	1:B:351:MET:HG3	1.96	0.46
1:C:340:ASP:O	1:C:413:THR:HA	2.15	0.46
1:E:430:LEU:HB3	1:E:434:VAL:HB	1.97	0.46
1:G:158:VAL:HG13	1:G:160:ARG:H	1.80	0.46
1:H:46:PRO:HD2	1:H:89:SER:O	2.15	0.46
1:D:135:SER:OG	1:D:324:ARG:NH2	2.42	0.46
1:E:223:VAL:O	1:E:224:VAL:HG12	2.15	0.46
1:E:452:ASN:HD21	1:E:455:LYS:HD2	1.80	0.46
1:H:313:GLU:CD	1:H:315:GLU:H	2.23	0.46
1:H:343:VAL:HG21	1:H:351:MET:HG3	1.97	0.46
1:B:366:ILE:HG22	1:B:381:PHE:HB2	1.97	0.46
1:E:69:ARG:NH2	1:E:72:GLY:HA3	2.30	0.46
1:E:106:VAL:HG11	1:E:117:LEU:HD11	1.95	0.46
1:F:37:TYR:HB3	1:F:80:ASN:ND2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:287:SER:HA	1:F:290:GLU:CD	2.41	0.46
1:G:170:VAL:HG13	1:G:202:LEU:O	2.15	0.46
1:G:258:LEU:O	1:G:261:VAL:HG12	2.14	0.46
1:G:343:VAL:HG21	1:G:351:MET:HG3	1.97	0.46
1:C:223:VAL:HG22	1:C:224:VAL:HG23	1.97	0.46
1:F:381:PHE:CE2	1:F:383:VAL:HG12	2.50	0.46
1:G:379:PRO:HB2	1:G:398:PHE:HE1	1.80	0.46
1:A:437:MET:HE1	1:B:178:LEU:HD21	1.96	0.46
1:B:283:LEU:O	1:B:289:GLN:HB3	2.16	0.46
1:B:355:ILE:HG22	1:B:401:ILE:HG12	1.96	0.46
1:C:423:MET:HG3	1:C:456:VAL:O	2.15	0.46
1:C:452:ASN:ND2	1:C:455:LYS:HD2	2.30	0.46
1:E:29:HIS:HB3	1:E:37:TYR:CG	2.50	0.46
1:E:167:GLU:HB3	1:E:207:GLU:HB3	1.97	0.46
1:G:253:ILE:HG23	1:G:276:LEU:HD22	1.98	0.46
1:H:180:ARG:HD3	1:H:185:GLY:HA3	1.96	0.46
1:B:16:GLN:OE1	1:B:92:ARG:NH1	2.48	0.46
1:E:250:LEU:HD12	1:E:278:LEU:O	2.16	0.46
1:A:280:ARG:HG2	1:A:281:SER:N	2.31	0.46
1:E:365:ARG:HG2	1:E:381:PHE:HE1	1.80	0.46
1:F:205:VAL:HG22	2:F:501:FAD:C6A	2.46	0.46
1:A:234:GLY:O	1:A:237:VAL:HG22	2.15	0.46
1:A:452:ASN:ND2	1:A:455:LYS:HD2	2.31	0.46
1:D:291:GLU:OE1	1:D:294:ARG:HB2	2.15	0.46
1:F:108:VAL:HG11	1:F:117:LEU:HD13	1.98	0.46
1:G:254:ASP:CG	1:G:368:ASN:H	2.23	0.46
1:C:250:LEU:HD23	1:C:373:GLY:HA2	1.97	0.46
2:C:501:FAD:C1'	2:C:501:FAD:H5'2	2.46	0.46
1:D:37:TYR:HB3	1:D:80:ASN:ND2	2.31	0.46
1:D:284:PRO:O	1:D:287:SER:OG	2.34	0.46
1:E:75:LEU:HD22	1:E:416:HIS:CE1	2.51	0.46
1:C:219:VAL:HG13	1:C:221:HIS:NE2	2.30	0.45
1:E:34:TRP:CE2	1:E:391:LYS:HD2	2.50	0.45
1:E:362:PHE:O	1:E:364:THR:HG23	2.16	0.45
1:F:323:ARG:HH21	1:F:371:HIS:CE1	2.34	0.45
1:G:277:LEU:HD23	1:G:277:LEU:HA	1.78	0.45
1:D:232:ASP:C	1:D:234:GLY:N	2.73	0.45
1:G:12:ILE:HG23	1:G:12:ILE:O	2.16	0.45
1:G:129:PRO:HG2	1:G:162:TYR:OH	2.16	0.45
1:G:255:ARG:HB2	1:G:274:GLU:HA	1.98	0.45
1:G:316:ALA:HA	1:G:319:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:THR:HG23	1:A:289:GLN:HE21	1.81	0.45
1:B:41:ALA:HB2	1:B:84:GLY:HA2	1.98	0.45
1:B:337:LEU:HD22	1:B:398:PHE:CD2	2.51	0.45
1:C:174:GLU:N	1:C:174:GLU:OE1	2.49	0.45
1:C:265:LYS:O	1:C:267:MET:HG3	2.16	0.45
1:E:131:ASP:OD1	1:E:131:ASP:N	2.49	0.45
1:E:452:ASN:ND2	1:E:455:LYS:HD2	2.32	0.45
1:F:245:ILE:HD13	1:F:291:GLU:OE2	2.16	0.45
1:G:287:SER:HA	1:G:290:GLU:HG2	1.97	0.45
1:C:16:GLN:HG3	1:C:45:ARG:O	2.16	0.45
1:C:260:ALA:HB1	1:C:333:LEU:HD11	1.99	0.45
1:E:62:ARG:HB2	1:E:64:VAL:HG12	1.97	0.45
1:F:7:GLU:OE1	1:F:58:ILE:HG23	2.17	0.45
1:F:160:ARG:NH1	1:F:161:ASP:OD1	2.50	0.45
1:A:299:PHE:O	1:A:304:ALA:HB2	2.16	0.45
1:A:374:ASP:HB2	1:B:183:ALA:HB3	1.98	0.45
1:A:378:HIS:CE1	1:A:415:GLU:OE2	2.70	0.45
1:B:38:ASP:OD1	1:B:39:ALA:N	2.40	0.45
1:C:131:ASP:OD1	1:C:131:ASP:N	2.49	0.45
1:E:292:ALA:HA	1:E:295:ILE:HG12	1.99	0.45
1:B:131:ASP:CG	1:B:324:ARG:HH22	2.25	0.45
1:C:224:VAL:CG2	1:C:299:PHE:HD2	2.29	0.45
1:D:224:VAL:HG11	1:D:306:TYR:CD2	2.51	0.45
1:D:224:VAL:HG22	1:D:310:SER:HB2	1.99	0.45
1:F:174:GLU:OE1	1:F:174:GLU:N	2.46	0.45
1:B:313:GLU:HG3	1:B:317:GLU:HG3	1.99	0.45
1:C:4:VAL:O	1:C:8:LEU:HD13	2.17	0.45
1:C:153:CYS:C	1:C:155:LYS:H	2.25	0.45
1:E:44:VAL:HG11	1:E:55:VAL:HG21	1.98	0.45
1:F:235:ARG:O	1:F:302:GLU:HG3	2.16	0.45
1:F:261:VAL:HG22	1:F:330:LEU:HD11	1.98	0.45
1:G:369:ILE:HG13	1:G:378:HIS:HB2	1.98	0.45
1:A:355:ILE:HD13	1:A:379:PRO:HB3	1.98	0.45
1:A:398:PHE:O	1:A:402:VAL:HG23	2.16	0.45
1:B:389:GLU:HG2	1:B:393:ARG:HG3	1.99	0.45
1:D:232:ASP:HA	1:D:235:ARG:H	1.81	0.45
1:H:330:LEU:HA	1:H:333:LEU:HB3	1.99	0.45
1:B:131:ASP:OD1	1:B:131:ASP:N	2.50	0.45
1:C:378:HIS:NE2	1:C:415:GLU:OE2	2.50	0.45
1:F:423:MET:HE2	1:F:458:ALA:HB2	1.98	0.45
1:G:347:ARG:HG2	1:G:408:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:GLU:OE1	1:C:263:GLU:N	2.49	0.44
1:D:282:ASP:OD1	1:D:282:ASP:N	2.50	0.44
1:E:232:ASP:CG	1:E:235:ARG:HB2	2.42	0.44
1:E:232:ASP:HA	1:E:234:GLY:H	1.82	0.44
1:E:337:LEU:HD22	1:E:398:PHE:CD2	2.52	0.44
1:F:180:ARG:NH1	1:F:182:THR:C	2.74	0.44
1:F:339:GLU:O	1:F:378:HIS:HA	2.16	0.44
1:B:156:TYR:HB3	1:B:162:TYR:OH	2.16	0.44
1:C:222:THR:HG21	1:C:316:ALA:HB1	1.99	0.44
1:C:389:GLU:O	1:C:392:ARG:N	2.50	0.44
1:F:270:SER:OG	1:F:271:ALA:N	2.51	0.44
1:F:442:LYS:NZ	1:F:446:ASP:OD2	2.47	0.44
1:H:412:VAL:HG11	1:H:426:ALA:HA	1.98	0.44
1:A:38:ASP:OD2	1:A:83:ARG:HG2	2.17	0.44
1:B:15:GLU:HG2	1:B:92:ARG:HH22	1.83	0.44
1:B:264:TRP:CZ3	1:B:325:LEU:HD23	2.51	0.44
1:B:265:LYS:O	1:B:267:MET:HG3	2.17	0.44
1:C:289:GLN:HA	1:C:292:ALA:HB3	1.99	0.44
1:D:263:GLU:N	1:D:263:GLU:OE1	2.50	0.44
1:F:43:VAL:HG22	1:F:87:VAL:HB	2.00	0.44
1:G:177:ARG:NH2	1:G:207:GLU:OE1	2.49	0.44
1:A:328:PRO:HD3	2:A:501:FAD:HM71	1.98	0.44
1:B:166:MET:HE1	1:B:205:VAL:HG22	1.99	0.44
1:C:340:ASP:OD1	1:C:376:ASN:ND2	2.39	0.44
1:C:395:LYS:O	1:C:399:GLU:HG3	2.17	0.44
1:E:52:VAL:HG23	1:E:93:MET:HE1	1.99	0.44
1:F:223:VAL:HG21	1:F:295:ILE:HG22	1.99	0.44
1:H:211:ARG:C	1:H:212:LEU:HD12	2.43	0.44
1:A:349:PRO:O	1:A:353:GLU:HG3	2.18	0.44
1:B:43:VAL:HG22	1:B:87:VAL:HB	1.99	0.44
1:B:97:LEU:O	1:B:98:GLU:HB2	2.17	0.44
1:C:289:GLN:HG2	1:C:293:ASP:HB2	2.00	0.44
1:C:411:THR:HG22	1:C:429:GLU:OE2	2.18	0.44
1:E:348:VAL:N	1:E:349:PRO:HD2	2.33	0.44
1:F:327:TYR:CE1	1:F:336:LEU:HB3	2.53	0.44
1:G:239:ALA:HB3	1:G:301:LYS:NZ	2.32	0.44
1:H:452:ASN:ND2	1:H:455:LYS:HG3	2.32	0.44
1:A:384:PRO:C	1:A:386:GLY:H	2.25	0.44
1:C:289:GLN:HE21	1:C:293:ASP:CB	2.28	0.44
1:D:106:VAL:HG13	1:D:212:LEU:HD21	1.99	0.44
1:D:135:SER:OG	1:D:136:PRO:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:343:VAL:HG11	1:E:351:MET:SD	2.58	0.44
1:F:132:PRO:O	1:F:135:SER:N	2.51	0.44
1:F:302:GLU:CD	1:F:303:LYS:H	2.25	0.44
1:F:388:GLU:O	1:F:390:ALA:N	2.50	0.44
1:H:166:MET:HE3	1:H:192:ALA:HB1	1.99	0.44
1:A:348:VAL:N	1:A:349:PRO:HD2	2.33	0.44
1:B:166:MET:HE2	1:B:168:ALA:HB2	1.99	0.44
1:B:455:LYS:O	1:B:457:PHE:N	2.48	0.44
1:D:38:ASP:OD2	1:D:83:ARG:N	2.50	0.44
1:E:365:ARG:NH1	1:E:382:ILE:HG22	2.32	0.44
1:E:378:HIS:NE2	1:E:415:GLU:OE2	2.51	0.44
1:F:15:GLU:O	1:F:15:GLU:HG2	2.18	0.44
1:G:133:ALA:HB1	2:G:501:FAD:H6	1.14	0.44
1:G:346:ALA:C	1:G:347:ARG:HD2	2.42	0.44
1:A:444:ALA:HB1	1:B:440:ALA:HB1	2.00	0.44
2:A:501:FAD:O4'	2:A:501:FAD:O2'	2.20	0.44
1:D:233:ALA:HB1	1:D:252:LEU:CG	2.48	0.44
1:E:355:ILE:HD13	1:E:401:ILE:HD12	1.99	0.44
1:G:95:ARG:NH1	1:G:97:LEU:HD22	2.33	0.44
1:G:144:VAL:HG13	1:G:196:VAL:HG22	1.99	0.44
1:C:133:ALA:HB3	2:C:501:FAD:C5X	2.48	0.44
1:E:395:LYS:O	1:E:399:GLU:HG3	2.18	0.44
1:F:127:TRP:CH2	1:F:216:ARG:HD2	2.53	0.44
1:F:261:VAL:HA	1:F:330:LEU:HD11	1.99	0.44
1:G:6:GLU:O	1:G:9:VAL:HG22	2.18	0.44
1:H:250:LEU:HB3	1:H:373:GLY:HA3	1.99	0.44
1:B:391:LYS:O	1:B:395:LYS:HG3	2.18	0.43
1:C:90:PHE:HD1	1:C:93:MET:HE3	1.83	0.43
1:C:365:ARG:O	1:C:365:ARG:HG3	2.18	0.43
1:D:232:ASP:HA	1:D:235:ARG:N	2.33	0.43
1:E:379:PRO:HB2	1:E:398:PHE:HE1	1.82	0.43
1:F:299:PHE:O	1:F:304:ALA:HB2	2.17	0.43
1:G:292:ALA:C	1:G:309:ARG:HH21	2.24	0.43
1:H:348:VAL:N	1:H:349:PRO:HD2	2.33	0.43
1:A:5:VAL:HG22	1:A:42:ALA:HB2	2.00	0.43
1:E:103:GLN:HG3	1:E:105:THR:HG23	2.00	0.43
1:F:312:ASP:CG	1:F:313:GLU:H	2.26	0.43
1:F:351:MET:HE1	1:F:401:ILE:HG23	1.98	0.43
1:G:12:ILE:HG12	1:G:51:ASP:CG	2.43	0.43
1:H:73:THR:C	2:H:501:FAD:HO3'	2.17	0.43
1:H:73:THR:C	2:H:501:FAD:O3'	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:VAL:HG13	1:B:43:VAL:O	2.18	0.43
1:D:158:VAL:HG13	1:D:160:ARG:H	1.83	0.43
1:G:298:CYS:HA	1:G:301:LYS:HE2	2.00	0.43
1:G:296:LEU:O	1:G:299:PHE:N	2.51	0.43
1:D:312:ASP:C	1:D:314:GLU:H	2.23	0.43
1:G:7:GLU:HG2	1:G:58:ILE:HD13	2.00	0.43
1:C:250:LEU:HG	1:C:372:ALA:HB3	1.99	0.43
1:C:259:GLN:NE2	1:C:263:GLU:OE2	2.52	0.43
1:E:325:LEU:HA	1:E:328:PRO:HD2	1.99	0.43
1:E:348:VAL:HG13	1:E:377:LEU:HD21	2.00	0.43
1:G:233:ALA:HB1	1:G:277:LEU:HD12	2.00	0.43
1:A:34:TRP:HH2	1:A:383:VAL:HG21	1.83	0.43
2:B:501:FAD:H1'2	2:B:501:FAD:H9	1.62	0.43
1:C:224:VAL:HA	1:C:308:VAL:H	1.84	0.43
1:C:396:GLN:O	1:C:400:VAL:HG22	2.19	0.43
1:C:452:ASN:HD21	1:C:455:LYS:HD2	1.82	0.43
2:C:501:FAD:H1'1	2:C:501:FAD:H9	1.57	0.43
1:D:232:ASP:CA	1:D:235:ARG:HB2	2.45	0.43
1:D:278:LEU:HD21	1:D:319:LEU:HD13	2.00	0.43
1:D:415:GLU:HB2	2:D:501:FAD:O2	2.18	0.43
1:E:211:ARG:HG2	1:E:212:LEU:N	2.33	0.43
1:F:340:ASP:CG	1:F:414:GLY:H	2.24	0.43
2:G:501:FAD:H8A	2:G:501:FAD:O5B	2.19	0.43
1:B:221:HIS:CE1	1:B:223:VAL:HG23	2.53	0.43
1:D:327:TYR:N	1:D:328:PRO:HD2	2.33	0.43
1:E:155:LYS:NZ	1:E:282:ASP:OD1	2.43	0.43
1:E:329:ALA:C	1:E:331:GLU:N	2.77	0.43
1:F:435:LEU:HD23	1:F:435:LEU:HA	1.91	0.43
1:B:219:VAL:HG21	1:B:283:LEU:H	1.83	0.43
1:B:348:VAL:N	1:B:349:PRO:HD2	2.34	0.43
1:B:406:LEU:HD21	1:B:429:GLU:HB2	2.01	0.43
1:C:255:ARG:NH2	1:C:274:GLU:HB2	2.33	0.43
1:D:391:LYS:HB3	1:D:391:LYS:HE3	1.89	0.43
1:E:392:ARG:O	1:E:396:GLN:HG2	2.19	0.43
1:F:255:ARG:O	1:F:258:LEU:N	2.52	0.43
1:H:57:ARG:HH21	1:H:58:ILE:HD11	1.83	0.43
1:A:417:GLY:HA2	1:B:186:VAL:CG2	2.48	0.43
1:A:46:PRO:HB2	1:A:93:MET:CE	2.49	0.42
1:A:55:VAL:O	1:A:59:CYS:SG	2.76	0.42
1:A:170:VAL:HG23	1:A:202:LEU:O	2.19	0.42
1:A:222:THR:HG22	1:A:223:VAL:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:ILE:H	1:B:366:ILE:HG13	1.60	0.42
1:D:27:TYR:O	1:D:87:VAL:HG11	2.19	0.42
1:D:289:GLN:O	1:D:289:GLN:HG2	2.19	0.42
1:G:230:LEU:HD11	1:G:252:LEU:HD21	2.01	0.42
1:G:255:ARG:HD2	1:G:256:PHE:CD1	2.54	0.42
1:B:72:GLY:HA2	2:B:501:FAD:O1A	2.19	0.42
1:F:337:LEU:O	1:F:380:LEU:HA	2.19	0.42
1:A:109:GLN:O	1:A:112:VAL:HG12	2.18	0.42
1:A:186:VAL:HG13	1:B:413:THR:HG23	2.01	0.42
1:D:166:MET:HE2	1:D:205:VAL:HG21	2.00	0.42
1:E:78:ALA:C	1:E:455:LYS:HZ3	2.28	0.42
1:F:366:ILE:HG12	1:F:398:PHE:CE1	2.54	0.42
1:G:131:ASP:OD1	1:G:131:ASP:N	2.53	0.42
1:H:251:GLU:OE2	1:H:371:HIS:ND1	2.49	0.42
1:A:144:VAL:HG13	1:A:196:VAL:HG22	2.00	0.42
1:B:329:ALA:C	1:B:331:GLU:N	2.74	0.42
1:C:283:LEU:HB2	1:C:287:SER:O	2.19	0.42
1:C:289:GLN:NE2	1:C:293:ASP:HB2	2.32	0.42
1:H:235:ARG:HA	1:H:238:ALA:HB3	2.02	0.42
1:B:278:LEU:N	1:B:278:LEU:HD12	2.35	0.42
1:D:402:VAL:HG11	1:D:412:VAL:HG23	2.00	0.42
1:F:376:ASN:HD21	1:F:415:GLU:CD	2.27	0.42
2:G:501:FAD:H1'2	2:G:501:FAD:H9	1.65	0.42
1:A:8:LEU:HD23	1:A:8:LEU:HA	1.90	0.42
1:C:154:VAL:HG12	1:C:374:ASP:HB3	2.00	0.42
1:E:371:HIS:HB2	1:E:376:ASN:HB3	2.01	0.42
1:F:8:LEU:HD22	1:F:58:ILE:HG21	2.01	0.42
1:F:328:PRO:N	2:F:501:FAD:C7M	2.83	0.42
1:G:69:ARG:NH2	1:G:72:GLY:HA3	2.34	0.42
1:A:252:LEU:HB3	1:A:370:ALA:HB3	2.01	0.42
1:B:371:HIS:HB2	1:B:376:ASN:HB3	2.01	0.42
1:D:255:ARG:N	1:D:274:GLU:O	2.52	0.42
1:D:327:TYR:HE1	1:D:336:LEU:HD22	1.83	0.42
1:F:128:TYR:CE1	1:F:210:LEU:HD13	2.55	0.42
1:A:131:ASP:OD1	1:A:131:ASP:N	2.53	0.42
1:A:242:ALA:HB2	1:B:102:VAL:HG13	2.02	0.42
1:B:131:ASP:OD2	1:B:324:ARG:NH2	2.52	0.42
1:C:167:GLU:HB3	1:C:207:GLU:HB3	2.02	0.42
1:C:415:GLU:HB2	2:C:501:FAD:C4	2.50	0.42
1:D:398:PHE:O	1:D:402:VAL:HG23	2.20	0.42
1:E:339:GLU:HG3	1:E:398:PHE:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:VAL:HB	1:F:212:LEU:HD11	2.02	0.42
1:G:378:HIS:NE2	1:G:415:GLU:OE2	2.48	0.42
1:A:397:ALA:O	1:A:401:ILE:HG12	2.20	0.42
1:A:406:LEU:HD23	1:A:406:LEU:HA	1.89	0.42
1:C:32:ALA:HB2	1:C:75:LEU:HA	2.00	0.42
1:E:227:PHE:HZ	1:E:277:LEU:HD22	1.83	0.42
1:E:253:ILE:HD12	1:E:323:ARG:HA	2.01	0.42
1:G:293:ASP:O	1:G:294:ARG:HB3	2.20	0.42
1:H:442:LYS:NZ	1:H:446:ASP:OD2	2.45	0.42
1:A:280:ARG:HG2	1:A:281:SER:H	1.84	0.42
1:B:248:SER:HB2	1:B:282:ASP:OD1	2.20	0.42
1:C:132:PRO:C	1:C:134:SER:N	2.78	0.42
1:D:131:ASP:OD1	1:D:131:ASP:N	2.52	0.42
1:D:233:ALA:HB1	1:D:252:LEU:HD21	2.02	0.42
1:D:390:ALA:HA	1:D:393:ARG:HD3	2.02	0.42
1:F:335:PRO:HD2	1:F:383:VAL:O	2.20	0.42
1:G:455:LYS:O	1:G:457:PHE:N	2.53	0.42
1:A:164:LEU:HD22	1:A:180:ARG:NH1	2.35	0.41
1:A:404:GLU:O	1:A:408:VAL:HG13	2.20	0.41
1:C:118:ARG:NH2	1:C:130:PRO:O	2.52	0.41
1:E:5:VAL:O	1:E:9:VAL:HG23	2.20	0.41
1:E:16:GLN:O	1:E:44:VAL:HA	2.20	0.41
1:E:50:ALA:O	1:E:54:GLU:HG2	2.20	0.41
1:E:283:LEU:O	1:E:284:PRO:C	2.63	0.41
1:F:286:THR:O	1:F:290:GLU:HG3	2.20	0.41
1:G:185:GLY:HA2	1:H:413:THR:O	2.20	0.41
1:G:293:ASP:N	1:G:309:ARG:HH21	2.17	0.41
1:H:142:GLY:O	1:H:146:THR:HG22	2.20	0.41
1:A:114:ASN:HB3	1:A:135:SER:O	2.21	0.41
1:A:136:PRO:HG2	1:A:137:TRP:CE3	2.55	0.41
1:D:27:TYR:HD2	1:D:43:VAL:HG11	1.85	0.41
1:G:182:THR:HG23	1:H:344:PRO:HA	2.02	0.41
1:G:183:ALA:HB3	1:H:374:ASP:OD1	2.20	0.41
2:H:501:FAD:N1	2:H:501:FAD:O2'	2.51	0.41
1:B:129:PRO:HG2	1:B:162:TYR:OH	2.19	0.41
1:E:106:VAL:HG13	1:E:108:VAL:HG13	2.02	0.41
1:F:360:GLU:O	1:F:362:PHE:N	2.53	0.41
1:G:255:ARG:HB2	1:G:274:GLU:HB3	2.02	0.41
1:G:347:ARG:HD2	1:G:347:ARG:N	2.34	0.41
1:A:90:PHE:HZ	1:A:204:LEU:HB3	1.85	0.41
1:A:235:ARG:HB2	1:A:302:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:GLY:HA2	1:B:186:VAL:HG21	2.02	0.41
1:B:296:LEU:O	1:B:300:GLU:OE1	2.38	0.41
1:E:215:LEU:O	1:E:217:ARG:HG2	2.20	0.41
1:E:296:LEU:HD21	1:E:309:ARG:HG3	2.03	0.41
1:F:347:ARG:HG2	1:F:408:VAL:HG13	2.01	0.41
1:G:8:LEU:HD23	1:G:8:LEU:HA	1.92	0.41
1:G:154:VAL:HG11	1:G:373:GLY:HA3	2.03	0.41
1:G:204:LEU:HD22	1:G:451:PHE:HE1	1.86	0.41
1:H:134:SER:OG	2:H:501:FAD:H9	2.11	0.41
1:C:133:ALA:HB3	2:C:501:FAD:N5	2.36	0.41
1:C:225:GLY:C	1:C:276:LEU:HD12	2.45	0.41
1:F:90:PHE:HD1	1:F:93:MET:HE3	1.86	0.41
1:F:259:GLN:O	1:F:259:GLN:HG3	2.20	0.41
1:G:133:ALA:HA	1:G:324:ARG:HH12	1.84	0.41
1:A:134:SER:O	1:A:134:SER:OG	2.37	0.41
1:A:155:LYS:HB2	1:A:246:VAL:HG11	2.03	0.41
1:B:297:GLU:HA	1:B:300:GLU:OE2	2.20	0.41
1:D:278:LEU:HD13	1:D:320:PHE:CD1	2.56	0.41
1:D:332:ARG:O	1:D:332:ARG:HG2	2.21	0.41
1:F:289:GLN:CD	1:F:309:ARG:HH22	2.27	0.41
1:G:203:GLY:HA2	1:G:451:PHE:CE1	2.56	0.41
1:A:20:ASP:O	1:A:23:VAL:HG12	2.20	0.41
1:A:384:PRO:C	1:A:386:GLY:N	2.79	0.41
1:B:118:ARG:HA	1:B:121:VAL:HG22	2.01	0.41
1:B:333:LEU:HB3	1:D:385:ALA:HB2	2.02	0.41
1:D:292:ALA:HA	1:D:295:ILE:HG12	2.03	0.41
1:G:155:LYS:HD2	1:G:248:SER:HA	2.02	0.41
1:B:226:TYR:CE1	1:B:276:LEU:HD13	2.56	0.41
1:B:297:GLU:O	1:B:301:LYS:HG3	2.21	0.41
1:B:388:GLU:HG2	1:B:389:GLU:N	2.35	0.41
1:C:348:VAL:N	1:C:349:PRO:HD2	2.36	0.41
1:D:423:MET:HE2	1:D:458:ALA:HB2	2.03	0.41
1:F:253:ILE:HG23	1:F:276:LEU:HD12	2.02	0.41
1:G:391:LYS:NZ	1:G:395:LYS:HD2	2.36	0.41
1:H:164:LEU:HD21	1:H:211:ARG:HB3	2.02	0.41
1:A:209:THR:O	1:A:210:LEU:HB2	2.21	0.41
1:A:369:ILE:HG13	1:A:378:HIS:HB2	2.03	0.41
1:B:18:VAL:HG11	1:B:45:ARG:NH1	2.36	0.41
1:C:9:VAL:HA	1:C:13:GLY:CA	2.46	0.41
1:C:158:VAL:HG13	1:C:160:ARG:H	1.86	0.41
1:C:227:PHE:HB3	1:C:228:ASP:H	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:GLY:O	1:D:349:PRO:HG3	2.21	0.41
1:G:133:ALA:C	1:G:324:ARG:HH22	2.29	0.41
1:A:7:GLU:OE1	1:A:58:ILE:HG23	2.21	0.41
1:A:233:ALA:N	1:A:302:GLU:OE2	2.54	0.41
1:B:308:VAL:C	1:B:310:SER:N	2.76	0.41
1:B:435:LEU:HD23	1:B:435:LEU:HA	1.94	0.41
1:D:24:MET:HE3	1:D:43:VAL:HG23	2.03	0.41
1:F:289:GLN:OE1	1:F:309:ARG:NH2	2.54	0.41
1:G:25:GLU:H	1:G:25:GLU:HG2	1.63	0.41
1:H:166:MET:HA	1:H:208:VAL:HA	2.03	0.41
1:F:4:VAL:HG22	1:F:62:ARG:HD2	2.02	0.40
1:F:78:ALA:O	1:F:455:LYS:NZ	2.54	0.40
1:F:347:ARG:O	1:F:351:MET:HB2	2.21	0.40
1:A:239:ALA:O	1:A:243:ALA:N	2.53	0.40
1:C:255:ARG:HB2	1:C:274:GLU:HG3	2.02	0.40
1:D:230:LEU:O	1:D:233:ALA:HB3	2.21	0.40
1:G:12:ILE:HA	1:G:12:ILE:HD12	1.79	0.40
1:A:245:ILE:HB	1:A:246:VAL:H	1.53	0.40
1:B:333:LEU:HB3	1:D:385:ALA:CB	2.52	0.40
1:C:134:SER:OG	1:C:138:SER:HB3	2.21	0.40
1:F:109:GLN:O	1:F:112:VAL:HG22	2.20	0.40
1:H:195:MET:HE2	1:H:195:MET:HB2	1.96	0.40
1:B:27:TYR:O	1:B:87:VAL:HG11	2.21	0.40
1:B:28:SER:HB3	1:B:40:PRO:HD3	2.03	0.40
1:C:18:VAL:HG13	1:C:43:VAL:O	2.22	0.40
1:C:310:SER:C	1:C:312:ASP:H	2.30	0.40
1:C:348:VAL:HG13	1:C:377:LEU:HD21	2.03	0.40
1:C:416:HIS:CD2	2:C:501:FAD:N5	2.89	0.40
1:F:363:ASP:CB	1:F:393:ARG:HH22	2.18	0.40
1:A:129:PRO:HG2	1:A:162:TYR:OH	2.22	0.40
1:A:132:PRO:O	1:A:135:SER:N	2.54	0.40
1:A:392:ARG:NH1	1:F:388:GLU:OE2	2.55	0.40
1:C:252:LEU:O	1:C:369:ILE:HA	2.22	0.40
1:E:355:ILE:HG12	1:E:355:ILE:H	1.65	0.40
1:F:114:ASN:OD1	1:F:132:PRO:HD2	2.21	0.40
1:F:365:ARG:O	1:F:381:PHE:HD1	2.05	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:GLU:O	1:E:95:ARG:NH2[1_465]	2.14	0.06

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	438/464 (94%)	371 (85%)	52 (12%)	15 (3%)	3	6
1	B	439/464 (95%)	385 (88%)	43 (10%)	11 (2%)	4	9
1	C	439/464 (95%)	385 (88%)	45 (10%)	9 (2%)	5	12
1	D	449/464 (97%)	390 (87%)	49 (11%)	10 (2%)	5	11
1	E	444/464 (96%)	378 (85%)	50 (11%)	16 (4%)	2	5
1	F	436/464 (94%)	374 (86%)	41 (9%)	21 (5%)	2	3
1	G	449/464 (97%)	388 (86%)	43 (10%)	18 (4%)	2	3
1	H	357/464 (77%)	319 (89%)	37 (10%)	1 (0%)	36	55
All	All	3451/3712 (93%)	2990 (87%)	360 (10%)	101 (3%)	3	8

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	TRP
1	A	224	VAL
1	B	266	ASN
1	B	309	ARG
1	B	363	ASP
1	C	14	ALA
1	C	133	ALA
1	D	34	TRP
1	D	224	VAL
1	D	310	SER
1	D	313	GLU
1	E	217	ARG

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Mol	Chain	Res	Type
1	E	220	GLU
1	E	224	VAL
1	E	242	ALA
1	E	285	GLY
1	E	309	ARG
1	E	385	ALA
1	F	305	VAL
1	F	311	THR
1	F	332	ARG
1	F	363	ASP
1	G	228	ASP
1	G	284	PRO
1	G	303	LYS
1	G	363	ASP
1	A	33	GLU
1	A	155	LYS
1	A	245	ILE
1	A	303	LYS
1	A	363	ASP
1	B	245	ILE
1	B	290	GLU
1	C	171	GLY
1	C	224	VAL
1	C	277	LEU
1	C	385	ALA
1	D	227	PHE
1	D	311	THR
1	E	216	ARG
1	E	226	TYR
1	E	284	PRO
1	F	13	GLY
1	F	216	ARG
1	F	235	ARG
1	F	309	ARG
1	F	361	ARG
1	F	387	ASP
1	F	389	GLU
1	G	5	VAL
1	G	33	GLU
1	G	34	TRP
1	G	245	ILE
1	G	274	GLU

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Mol	Chain	Res	Type
1	G	285	GLY
1	H	14	ALA
1	A	210	LEU
1	A	307	ALA
1	A	385	ALA
1	C	235	ARG
1	E	14	ALA
1	E	219	VAL
1	F	248	SER
1	F	265	LYS
1	F	270	SER
1	G	229	SER
1	A	133	ALA
1	A	233	ALA
1	D	266	ASN
1	E	235	ARG
1	F	278	LEU
1	G	264	TRP
1	G	304	ALA
1	A	235	ARG
1	A	296	LEU
1	A	304	ALA
1	B	277	LEU
1	B	291	GLU
1	B	310	SER
1	D	14	ALA
1	D	303	LYS
1	E	227	PHE
1	F	14	ALA
1	F	182	THR
1	F	306	TYR
1	F	327	TYR
1	G	98	GLU
1	G	310	SER
1	B	235	ARG
1	B	307	ALA
1	D	385	ALA
1	E	425	GLY
1	F	133	ALA
1	G	230	LEU
1	G	266	ASN
1	G	385	ALA

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Mol	Chain	Res	Type
1	C	219	VAL
1	C	225	GLY
1	B	225	GLY
1	E	245	ILE
1	F	4	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	334/349 (96%)	314 (94%)	20 (6%)	17	36
1	B	336/349 (96%)	314 (94%)	22 (6%)	15	32
1	C	336/349 (96%)	312 (93%)	24 (7%)	13	29
1	D	339/349 (97%)	320 (94%)	19 (6%)	19	40
1	E	337/349 (97%)	314 (93%)	23 (7%)	14	31
1	F	332/349 (95%)	317 (96%)	15 (4%)	24	48
1	G	339/349 (97%)	307 (91%)	32 (9%)	8	18
1	H	271/349 (78%)	261 (96%)	10 (4%)	30	55
All	All	2624/2792 (94%)	2459 (94%)	165 (6%)	16	34

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	VAL
1	A	75	LEU
1	A	108	VAL
1	A	154	VAL
1	A	175	VAL
1	A	181	THR
1	A	186	VAL
1	A	208	VAL
1	A	215	LEU
1	A	223	VAL

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Mol	Chain	Res	Type
1	A	224	VAL
1	A	228	ASP
1	A	263	GLU
1	A	317	GLU
1	A	324	ARG
1	A	377	LEU
1	A	391	LYS
1	A	408	VAL
1	A	411	THR
1	A	412	VAL
1	B	4	VAL
1	B	12	ILE
1	B	18	VAL
1	B	23	VAL
1	B	67	VAL
1	B	97	LEU
1	B	112	VAL
1	B	170	VAL
1	B	176	VAL
1	B	186	VAL
1	B	187	THR
1	B	219	VAL
1	B	222	THR
1	B	223	VAL
1	B	224	VAL
1	B	295	ILE
1	B	296	LEU
1	B	311	THR
1	B	366	ILE
1	B	377	LEU
1	B	411	THR
1	B	450	ILE
1	C	4	VAL
1	C	18	VAL
1	C	25	GLU
1	C	64	VAL
1	C	67	VAL
1	C	106	VAL
1	C	153	CYS
1	C	175	VAL
1	C	186	VAL
1	C	187	THR

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Mol	Chain	Res	Type
1	C	222	THR
1	C	224	VAL
1	C	235	ARG
1	C	264	TRP
1	C	275	VAL
1	C	305	VAL
1	C	311	THR
1	C	351	MET
1	C	368	ASN
1	C	369	ILE
1	C	388	GLU
1	C	402	VAL
1	C	411	THR
1	C	423	MET
1	D	12	ILE
1	D	64	VAL
1	D	67	VAL
1	D	108	VAL
1	D	146	THR
1	D	166	MET
1	D	175	VAL
1	D	187	THR
1	D	215	LEU
1	D	228	ASP
1	D	237	VAL
1	D	265	LYS
1	D	266	ASN
1	D	308	VAL
1	D	311	THR
1	D	355	ILE
1	D	382	ILE
1	D	388	GLU
1	D	435	LEU
1	E	12	ILE
1	E	19	THR
1	E	24	MET
1	E	64	VAL
1	E	75	LEU
1	E	106	VAL
1	E	181	THR
1	E	186	VAL
1	E	215	LEU

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Mol	Chain	Res	Type
1	E	223	VAL
1	E	224	VAL
1	E	227	PHE
1	E	228	ASP
1	E	245	ILE
1	E	263	GLU
1	E	274	GLU
1	E	283	LEU
1	E	287	SER
1	E	308	VAL
1	E	313	GLU
1	E	351	MET
1	E	355	ILE
1	E	411	THR
1	F	18	VAL
1	F	113	VAL
1	F	170	VAL
1	F	175	VAL
1	F	187	THR
1	F	220	GLU
1	F	221	HIS
1	F	276	LEU
1	F	302	GLU
1	F	311	THR
1	F	333	LEU
1	F	347	ARG
1	F	351	MET
1	F	355	ILE
1	F	408	VAL
1	G	9	VAL
1	G	25	GLU
1	G	64	VAL
1	G	96	VAL
1	G	97	LEU
1	G	154	VAL
1	G	159	THR
1	G	166	MET
1	G	170	VAL
1	G	182	THR
1	G	186	VAL
1	G	187	THR
1	G	204	LEU

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Mol	Chain	Res	Type
1	G	208	VAL
1	G	224	VAL
1	G	228	ASP
1	G	240	VAL
1	G	246	VAL
1	G	248	SER
1	G	253	ILE
1	G	261	VAL
1	G	266	ASN
1	G	275	VAL
1	G	277	LEU
1	G	283	LEU
1	G	295	ILE
1	G	300	GLU
1	G	303	LYS
1	G	305	VAL
1	G	355	ILE
1	G	391	LYS
1	G	411	THR
1	H	28	SER
1	H	67	VAL
1	H	75	LEU
1	H	175	VAL
1	H	194	LEU
1	H	208	VAL
1	H	308	VAL
1	H	356	GLU
1	H	380	LEU
1	H	412	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	A	289	GLN
1	A	376	ASN
1	B	109	GLN
1	B	114	ASN
1	C	143	ASN
1	C	289	GLN
1	D	371	HIS
1	D	376	ASN

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Mol	Chain	Res	Type
1	E	103	GLN
1	E	259	GLN
1	E	416	HIS
1	F	221	HIS
1	F	376	ASN
1	G	143	ASN
1	G	416	HIS
1	G	433	HIS
1	H	94	ASN
1	H	104	GLN
1	H	109	GLN
1	H	376	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAD	D	501	-	58,58,58	1.92	15 (25%)	85,89,89	1.96	28 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	F	501	3	58,58,58	1.97	18 (31%)	85,89,89	1.95	23 (27%)
2	FAD	B	501	-	58,58,58	1.93	17 (29%)	85,89,89	1.69	24 (28%)
2	FAD	C	501	-	58,58,58	2.24	23 (39%)	85,89,89	2.15	27 (31%)
2	FAD	G	501	3	58,58,58	1.84	18 (31%)	85,89,89	1.98	25 (29%)
2	FAD	A	501	3	58,58,58	2.08	20 (34%)	85,89,89	2.23	29 (34%)
2	FAD	H	501	3	58,58,58	1.96	14 (24%)	85,89,89	1.79	22 (25%)
2	FAD	E	501	-	58,58,58	2.03	17 (29%)	85,89,89	2.26	34 (40%)

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	D	501	-	-	14/34/50/50	0/6/6/6
2	FAD	F	501	3	-	14/34/50/50	0/6/6/6
2	FAD	B	501	-	-	17/34/50/50	0/6/6/6
2	FAD	C	501	-	-	21/34/50/50	0/6/6/6
2	FAD	G	501	3	-	12/34/50/50	0/6/6/6
2	FAD	A	501	3	-	9/34/50/50	0/6/6/6
2	FAD	H	501	3	-	11/34/50/50	0/6/6/6
2	FAD	E	501	-	-	13/34/50/50	0/6/6/6

All (142) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	FAD	P-O3P	-6.56	1.52	1.59
2	H	501	FAD	P-O3P	-6.03	1.53	1.59
2	A	501	FAD	P-O3P	-5.65	1.53	1.59
2	F	501	FAD	C5A-N7A	-5.13	1.29	1.39
2	B	501	FAD	C5A-N7A	-5.07	1.29	1.39
2	C	501	FAD	PA-O3P	-5.04	1.54	1.59
2	E	501	FAD	C5X-N5	-5.04	1.30	1.39
2	F	501	FAD	P-O3P	-4.92	1.54	1.59
2	D	501	FAD	P-O3P	-4.83	1.54	1.59
2	B	501	FAD	C4A-N9A	-4.81	1.27	1.37
2	H	501	FAD	C5A-N7A	-4.76	1.30	1.39
2	H	501	FAD	C9A-C5X	4.64	1.48	1.41
2	E	501	FAD	C4-N3	-4.51	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	FAD	P-O3P	-4.51	1.54	1.59
2	H	501	FAD	PA-O3P	-4.38	1.54	1.59
2	F	501	FAD	C4A-N9A	-4.34	1.28	1.37
2	E	501	FAD	C5A-N7A	-4.31	1.31	1.39
2	A	501	FAD	C4A-N9A	-4.27	1.28	1.37
2	E	501	FAD	C4A-N9A	-4.26	1.28	1.37
2	D	501	FAD	C9A-C5X	4.21	1.48	1.41
2	C	501	FAD	C4A-N9A	-4.18	1.29	1.37
2	C	501	FAD	C5A-N7A	-3.99	1.31	1.39
2	E	501	FAD	C8-C7	3.95	1.50	1.40
2	B	501	FAD	P-O3P	-3.88	1.55	1.59
2	D	501	FAD	C4-N3	-3.82	1.31	1.38
2	G	501	FAD	C5A-N7A	-3.82	1.32	1.39
2	F	501	FAD	C9A-C5X	3.82	1.47	1.41
2	B	501	FAD	C8A-N9A	-3.76	1.31	1.37
2	D	501	FAD	C5A-N7A	-3.75	1.32	1.39
2	D	501	FAD	C4A-N9A	-3.74	1.29	1.37
2	A	501	FAD	C9A-C5X	3.72	1.47	1.41
2	A	501	FAD	C4-N3	-3.66	1.32	1.38
2	H	501	FAD	C4A-N9A	-3.62	1.30	1.37
2	F	501	FAD	C8A-N9A	-3.58	1.31	1.37
2	F	501	FAD	C4-N3	-3.50	1.32	1.38
2	D	501	FAD	C8A-N9A	-3.49	1.31	1.37
2	G	501	FAD	C5X-N5	-3.45	1.33	1.39
2	C	501	FAD	C2-N3	-3.40	1.31	1.39
2	G	501	FAD	P-O3P	-3.37	1.55	1.59
2	B	501	FAD	C5X-N5	-3.37	1.33	1.39
2	A	501	FAD	P-O2P	-3.37	1.39	1.55
2	A	501	FAD	C2A-N1A	-3.36	1.28	1.33
2	C	501	FAD	C8A-N9A	-3.36	1.31	1.37
2	H	501	FAD	C8A-N9A	-3.35	1.31	1.37
2	A	501	FAD	C8A-N9A	-3.35	1.31	1.37
2	G	501	FAD	C2-N3	-3.35	1.31	1.39
2	B	501	FAD	C4-N3	-3.34	1.32	1.38
2	G	501	FAD	C9A-C5X	3.32	1.46	1.41
2	C	501	FAD	C4-N3	-3.27	1.32	1.38
2	G	501	FAD	C4-N3	-3.27	1.32	1.38
2	H	501	FAD	C5X-N5	-3.22	1.33	1.39
2	H	501	FAD	O4B-C4B	-3.20	1.37	1.45
2	E	501	FAD	C9A-C5X	3.17	1.46	1.41
2	H	501	FAD	C4-N3	-3.12	1.33	1.38
2	E	501	FAD	C8A-N9A	-3.10	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	FAD	P-O2P	-3.08	1.41	1.55
2	A	501	FAD	C5A-N7A	-3.06	1.33	1.39
2	D	501	FAD	C2-N3	-3.05	1.32	1.39
2	A	501	FAD	C2'-C3'	-3.05	1.48	1.53
2	A	501	FAD	C2-N3	-3.03	1.32	1.39
2	B	501	FAD	P-O2P	-3.03	1.41	1.55
2	G	501	FAD	C2-N1	-3.03	1.29	1.36
2	F	501	FAD	PA-O3P	-3.03	1.56	1.59
2	C	501	FAD	PA-O1A	-3.03	1.40	1.50
2	A	501	FAD	P-O1P	-3.01	1.40	1.50
2	B	501	FAD	C9A-C5X	3.00	1.46	1.41
2	G	501	FAD	C8A-N9A	-2.96	1.32	1.37
2	C	501	FAD	C5X-N5	-2.96	1.34	1.39
2	D	501	FAD	C5X-N5	-2.95	1.34	1.39
2	G	501	FAD	PA-O3P	-2.94	1.56	1.59
2	F	501	FAD	P-O1P	-2.93	1.40	1.50
2	G	501	FAD	C4A-N9A	-2.88	1.31	1.37
2	F	501	FAD	C5X-N5	-2.88	1.34	1.39
2	C	501	FAD	C1'-C2'	-2.87	1.48	1.52
2	E	501	FAD	PA-O3P	-2.85	1.56	1.59
2	H	501	FAD	C2-N3	-2.85	1.32	1.39
2	H	501	FAD	P-O2P	-2.81	1.42	1.55
2	D	501	FAD	C6-C7	-2.78	1.35	1.39
2	E	501	FAD	C1'-C2'	-2.77	1.48	1.52
2	F	501	FAD	C2-N1	-2.77	1.30	1.36
2	B	501	FAD	C9A-N10	-2.74	1.36	1.41
2	A	501	FAD	C5X-N5	-2.73	1.34	1.39
2	D	501	FAD	PA-O3P	-2.70	1.56	1.59
2	C	501	FAD	C4'-C3'	-2.68	1.48	1.53
2	B	501	FAD	C2-N3	-2.67	1.33	1.39
2	C	501	FAD	C5'-C4'	-2.67	1.48	1.51
2	G	501	FAD	O4B-C4B	-2.67	1.39	1.45
2	C	501	FAD	C5A-C4A	2.63	1.43	1.39
2	D	501	FAD	C8-C7	2.63	1.47	1.40
2	A	501	FAD	PA-O3P	-2.62	1.56	1.59
2	E	501	FAD	C2'-C3'	-2.60	1.48	1.53
2	B	501	FAD	C2'-C3'	-2.60	1.48	1.53
2	G	501	FAD	P-O2P	-2.57	1.43	1.55
2	F	501	FAD	C2-N3	-2.57	1.33	1.39
2	C	501	FAD	P-O1P	-2.55	1.42	1.50
2	A	501	FAD	C2A-N3A	-2.53	1.29	1.33
2	H	501	FAD	C8-C7	2.53	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	FAD	P-O2P	-2.52	1.43	1.55
2	A	501	FAD	C2-N1	-2.50	1.31	1.36
2	H	501	FAD	P-O1P	-2.48	1.42	1.50
2	C	501	FAD	P-O2P	-2.48	1.43	1.55
2	C	501	FAD	C9A-N10	-2.47	1.36	1.41
2	A	501	FAD	PA-O2A	-2.47	1.43	1.55
2	C	501	FAD	O4B-C4B	-2.47	1.39	1.45
2	E	501	FAD	P-O5'	-2.47	1.49	1.59
2	B	501	FAD	C2-N1	-2.46	1.31	1.36
2	A	501	FAD	C5A-C6A	2.45	1.47	1.41
2	C	501	FAD	O5B-C5B	-2.41	1.35	1.44
2	F	501	FAD	O4B-C4B	-2.39	1.39	1.45
2	D	501	FAD	O4B-C4B	-2.39	1.39	1.45
2	B	501	FAD	P-O1P	-2.38	1.42	1.50
2	D	501	FAD	C5A-C4A	2.38	1.43	1.39
2	F	501	FAD	C6A-N1A	-2.34	1.29	1.35
2	G	501	FAD	C2A-N1A	-2.33	1.29	1.33
2	E	501	FAD	C5A-C4A	2.33	1.43	1.39
2	E	501	FAD	C2-N3	-2.31	1.33	1.39
2	B	501	FAD	O4B-C4B	-2.29	1.39	1.45
2	A	501	FAD	C6A-N1A	-2.29	1.29	1.35
2	F	501	FAD	PA-O2A	-2.29	1.44	1.55
2	G	501	FAD	C2'-C3'	-2.28	1.49	1.53
2	B	501	FAD	PA-O2A	-2.22	1.45	1.55
2	F	501	FAD	C2B-C3B	-2.21	1.47	1.53
2	A	501	FAD	C4A-N3A	-2.20	1.30	1.34
2	D	501	FAD	C2'-C3'	-2.19	1.49	1.53
2	B	501	FAD	C4A-N3A	-2.18	1.30	1.34
2	H	501	FAD	C5A-C4A	2.18	1.43	1.39
2	A	501	FAD	C5A-C4A	2.17	1.43	1.39
2	C	501	FAD	C6-C5X	-2.17	1.36	1.40
2	C	501	FAD	P-O5'	-2.16	1.50	1.59
2	G	501	FAD	PA-O1A	-2.16	1.43	1.50
2	E	501	FAD	P-O1P	-2.15	1.43	1.50
2	C	501	FAD	PA-O2A	-2.11	1.45	1.55
2	F	501	FAD	C8-C7	2.10	1.46	1.40
2	G	501	FAD	C9A-N10	-2.10	1.37	1.41
2	B	501	FAD	C2A-N3A	-2.06	1.30	1.33
2	D	501	FAD	P-O2P	-2.05	1.45	1.55
2	F	501	FAD	PA-O1A	-2.04	1.43	1.50
2	G	501	FAD	C2B-C3B	-2.03	1.47	1.53
2	E	501	FAD	PA-O2A	-2.02	1.46	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	FAD	C1'-C2'	-2.02	1.49	1.52
2	C	501	FAD	C8-C7	2.01	1.45	1.40
2	C	501	FAD	C6A-N1A	-2.01	1.30	1.35

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	FAD	C5'-C4'-C3'	-9.13	94.99	112.22
2	E	501	FAD	C5X-N5-C4X	7.03	129.47	118.09
2	F	501	FAD	C5A-C4A-N3A	-6.80	117.35	126.72
2	A	501	FAD	C5A-C4A-N3A	-6.20	118.17	126.72
2	G	501	FAD	C5A-C4A-N3A	-6.15	118.25	126.72
2	E	501	FAD	C9A-C5X-N5	-6.10	115.98	122.45
2	A	501	FAD	C4A-C5A-N7A	-6.03	103.68	110.58
2	G	501	FAD	N3A-C4A-N9A	5.51	136.54	127.17
2	D	501	FAD	C5A-C4A-N3A	-5.43	119.24	126.72
2	H	501	FAD	C5A-C4A-N3A	-5.38	119.31	126.72
2	A	501	FAD	C6A-C5A-N7A	5.38	142.46	132.09
2	H	501	FAD	N3A-C4A-N9A	5.05	135.75	127.17
2	A	501	FAD	C2A-N3A-C4A	5.05	124.16	111.83
2	A	501	FAD	C5A-C4A-N9A	4.98	111.24	105.81
2	E	501	FAD	C5A-C4A-N3A	-4.94	119.92	126.72
2	F	501	FAD	O2-C2-N1	-4.70	113.99	121.80
2	D	501	FAD	O2-C2-N1	-4.66	114.05	121.80
2	F	501	FAD	C4X-C10-N10	4.60	123.07	116.48
2	C	501	FAD	C10-N1-C2	4.60	126.80	116.85
2	G	501	FAD	C2A-N3A-C4A	4.54	122.93	111.83
2	A	501	FAD	C2B-C1B-N9A	4.45	124.36	113.30
2	C	501	FAD	C4-C4X-N5	4.40	124.29	118.21
2	B	501	FAD	C5A-C4A-N3A	-4.36	120.71	126.72
2	A	501	FAD	C4'-C3'-C2'	-4.32	106.39	113.57
2	G	501	FAD	N3A-C2A-N1A	-4.31	122.06	128.58
2	A	501	FAD	N3A-C2A-N1A	-4.28	122.11	128.58
2	F	501	FAD	O3P-PA-O1A	-4.27	97.85	110.70
2	B	501	FAD	O2-C2-N1	-4.24	114.75	121.80
2	D	501	FAD	C4X-C10-N10	4.13	122.39	116.48
2	E	501	FAD	N3A-C2A-N1A	-4.10	122.38	128.58
2	E	501	FAD	C5'-C4'-C3'	-4.09	104.50	112.22
2	C	501	FAD	C5A-C4A-N3A	-4.04	121.16	126.72
2	F	501	FAD	N3A-C4A-N9A	4.01	133.98	127.17
2	H	501	FAD	N3A-C2A-N1A	-4.00	122.52	128.58
2	F	501	FAD	C4A-C5A-N7A	-3.96	106.06	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	FAD	N3A-C2A-N1A	-3.96	122.59	128.58
2	E	501	FAD	C6-C5X-C9A	3.94	124.47	119.05
2	D	501	FAD	C2A-N3A-C4A	3.94	121.46	111.83
2	G	501	FAD	C5X-C9A-N10	3.93	121.52	117.97
2	E	501	FAD	C2A-N3A-C4A	3.88	121.32	111.83
2	D	501	FAD	N3A-C4A-N9A	3.87	133.76	127.17
2	D	501	FAD	C4A-C5A-N7A	-3.84	106.19	110.58
2	C	501	FAD	C5B-C4B-C3B	-3.82	101.47	115.21
2	G	501	FAD	O2-C2-N1	-3.80	115.49	121.80
2	D	501	FAD	C4-N3-C2	-3.79	118.92	125.64
2	E	501	FAD	O5'-P-O1P	-3.77	93.98	108.94
2	E	501	FAD	N3A-C4A-N9A	3.76	133.56	127.17
2	F	501	FAD	C2A-N3A-C4A	3.73	120.93	111.83
2	E	501	FAD	O2-C2-N1	-3.70	115.65	121.80
2	H	501	FAD	C2A-N3A-C4A	3.68	120.82	111.83
2	H	501	FAD	C4A-N9A-C8A	3.62	109.54	105.74
2	F	501	FAD	O4'-C4'-C5'	-3.59	102.06	109.99
2	D	501	FAD	N3A-C2A-N1A	-3.58	123.16	128.58
2	C	501	FAD	C4X-C10-N1	-3.58	115.81	124.59
2	B	501	FAD	C2A-N3A-C4A	3.55	120.51	111.83
2	A	501	FAD	O4B-C1B-N9A	-3.53	101.31	108.09
2	F	501	FAD	C9A-N10-C10	-3.52	115.38	120.75
2	A	501	FAD	C4-C4X-N5	3.51	123.05	118.21
2	C	501	FAD	C4A-C5A-N7A	-3.47	106.62	110.58
2	G	501	FAD	C4A-N9A-C8A	3.46	109.38	105.74
2	E	501	FAD	C4'-C3'-C2'	-3.41	107.89	113.57
2	G	501	FAD	O4-C4-C4X	-3.36	117.67	126.53
2	C	501	FAD	N3A-C2A-N1A	-3.33	123.54	128.58
2	F	501	FAD	C4X-C10-N1	-3.31	116.46	124.59
2	D	501	FAD	O3P-PA-O1A	-3.25	100.92	110.70
2	G	501	FAD	C10-N1-C2	3.24	123.87	116.85
2	A	501	FAD	O3B-C3B-C4B	-3.23	101.80	111.08
2	A	501	FAD	O2-C2-N1	-3.22	116.45	121.80
2	E	501	FAD	C10-C4X-N5	-3.21	118.25	124.81
2	F	501	FAD	C10-N1-C2	3.19	123.75	116.85
2	C	501	FAD	O2A-PA-O3P	3.18	115.88	107.27
2	C	501	FAD	O5'-C5'-C4'	3.18	117.86	109.36
2	E	501	FAD	C2'-C1'-N10	-3.15	95.32	110.20
2	C	501	FAD	O5B-PA-O1A	-3.15	96.46	108.94
2	E	501	FAD	O3B-C3B-C4B	-3.11	102.14	111.08
2	G	501	FAD	O3B-C3B-C4B	-3.10	102.17	111.08
2	H	501	FAD	C4'-C3'-C2'	-3.08	108.44	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	FAD	C1'-C2'-C3'	3.07	117.98	109.66
2	B	501	FAD	C4A-C5A-N7A	-3.07	107.08	110.58
2	C	501	FAD	C2A-N1A-C6A	3.05	123.74	118.73
2	D	501	FAD	C4A-N9A-C8A	3.02	108.91	105.74
2	H	501	FAD	C9A-N10-C10	-3.01	116.17	120.75
2	D	501	FAD	C5B-C4B-C3B	-3.00	104.41	115.21
2	C	501	FAD	C1'-N10-C9A	-2.99	114.81	120.63
2	C	501	FAD	C2A-N3A-C4A	2.98	119.12	111.83
2	C	501	FAD	O2P-P-O3P	2.98	115.32	107.27
2	H	501	FAD	O2-C2-N1	-2.97	116.86	121.80
2	G	501	FAD	O3P-PA-O1A	-2.97	101.77	110.70
2	A	501	FAD	O2'-C2'-C3'	-2.97	102.30	109.25
2	E	501	FAD	C4X-C10-N1	-2.97	117.31	124.59
2	G	501	FAD	C4X-C10-N1	-2.96	117.33	124.59
2	D	501	FAD	N3-C2-N1	2.92	125.71	119.50
2	D	501	FAD	C4X-C10-N1	-2.92	117.43	124.59
2	C	501	FAD	C2'-C1'-N10	-2.92	96.41	110.20
2	D	501	FAD	C4'-C3'-C2'	-2.91	108.73	113.57
2	C	501	FAD	C6A-C5A-N7A	2.89	137.67	132.09
2	D	501	FAD	C6A-C5A-N7A	2.89	137.67	132.09
2	C	501	FAD	C5X-N5-C4X	2.89	122.77	118.09
2	B	501	FAD	C4A-N9A-C1B	-2.89	119.87	126.63
2	A	501	FAD	C1B-N9A-C8A	2.88	133.49	127.09
2	E	501	FAD	C8M-C8-C9	-2.88	114.50	119.57
2	A	501	FAD	C4X-C10-N10	2.88	120.60	116.48
2	H	501	FAD	O3P-PA-O1A	-2.86	102.09	110.70
2	B	501	FAD	C4'-C3'-C2'	-2.83	108.86	113.57
2	G	501	FAD	C2B-C1B-N9A	-2.81	106.31	113.30
2	G	501	FAD	C4'-C3'-C2'	-2.79	108.93	113.57
2	B	501	FAD	C4-C4X-N5	2.79	122.06	118.21
2	E	501	FAD	C4-N3-C2	-2.77	120.72	125.64
2	B	501	FAD	N3A-C4A-N9A	2.77	131.88	127.17
2	B	501	FAD	C4X-C10-N1	-2.77	117.81	124.59
2	A	501	FAD	C10-N1-C2	2.75	122.81	116.85
2	C	501	FAD	C4X-C4-N3	2.73	120.20	113.25
2	A	501	FAD	C4X-C10-N1	-2.73	117.90	124.59
2	C	501	FAD	C10-C4X-N5	-2.73	119.24	124.81
2	C	501	FAD	N3A-C4A-N9A	2.72	131.79	127.17
2	E	501	FAD	O2P-P-O1P	2.72	125.08	112.44
2	H	501	FAD	C4X-C10-N10	2.71	120.36	116.48
2	D	501	FAD	O4'-C4'-C3'	-2.70	102.94	109.25
2	A	501	FAD	O2A-PA-O3P	2.69	114.56	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	FAD	O5'-C5'-C4'	2.69	116.55	109.36
2	F	501	FAD	N3A-C2A-N1A	-2.65	124.57	128.58
2	G	501	FAD	N9A-C8A-N7A	-2.64	110.19	113.94
2	C	501	FAD	O3P-PA-O1A	-2.63	102.80	110.70
2	D	501	FAD	C9A-N10-C10	-2.62	116.76	120.75
2	F	501	FAD	C5A-C4A-N9A	2.62	108.66	105.81
2	D	501	FAD	C4-C4X-N5	2.61	121.81	118.21
2	H	501	FAD	C2'-C1'-N10	2.61	122.53	110.20
2	A	501	FAD	C4A-N9A-C1B	-2.60	120.56	126.63
2	B	501	FAD	C6A-C5A-N7A	2.59	137.09	132.09
2	E	501	FAD	O2A-PA-O3P	2.59	114.27	107.27
2	B	501	FAD	C10-N1-C2	2.58	122.44	116.85
2	D	501	FAD	C5A-N7A-C8A	2.58	107.50	103.45
2	G	501	FAD	C9-C9A-N10	-2.55	118.42	121.85
2	H	501	FAD	N9A-C8A-N7A	-2.54	110.33	113.94
2	H	501	FAD	C4X-C10-N1	-2.54	118.36	124.59
2	G	501	FAD	C6A-C5A-N7A	2.52	136.94	132.09
2	D	501	FAD	N9A-C8A-N7A	-2.49	110.40	113.94
2	B	501	FAD	N9A-C8A-N7A	-2.49	110.40	113.94
2	E	501	FAD	O4-C4-C4X	-2.49	119.97	126.53
2	B	501	FAD	C4A-N9A-C8A	2.48	108.35	105.74
2	D	501	FAD	C2B-C1B-N9A	-2.48	107.13	113.30
2	H	501	FAD	O4-C4-C4X	-2.48	119.98	126.53
2	F	501	FAD	O2-C2-N3	2.48	123.34	118.58
2	H	501	FAD	O2P-P-O3P	2.46	113.93	107.27
2	A	501	FAD	C6A-C5A-C4A	-2.45	113.83	117.18
2	A	501	FAD	C5A-N7A-C8A	2.42	107.25	103.45
2	F	501	FAD	O2A-PA-O1A	2.42	123.68	112.44
2	D	501	FAD	C4X-C4-N3	2.41	119.39	113.25
2	D	501	FAD	O4-C4-C4X	-2.39	120.22	126.53
2	B	501	FAD	C5'-C4'-C3'	-2.39	107.72	112.22
2	B	501	FAD	C4X-C10-N10	2.38	119.89	116.48
2	G	501	FAD	C5A-N7A-C8A	2.38	107.19	103.45
2	E	501	FAD	O5'-C5'-C4'	-2.37	103.03	109.36
2	G	501	FAD	C9A-N10-C10	-2.37	117.14	120.75
2	C	501	FAD	N10-C10-N1	2.37	125.48	118.51
2	C	501	FAD	C4A-N9A-C8A	2.35	108.21	105.74
2	A	501	FAD	O3'-C3'-C4'	2.35	114.27	108.93
2	H	501	FAD	C5X-C9A-N10	2.34	120.08	117.97
2	F	501	FAD	C4-C4X-N5	2.34	121.44	118.21
2	H	501	FAD	O2'-C2'-C3'	-2.33	103.78	109.25
2	H	501	FAD	C5A-C6A-N6A	-2.33	117.51	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	501	FAD	C4X-C4-N3	2.31	119.14	113.25
2	D	501	FAD	O3P-P-O1P	-2.31	103.75	110.70
2	E	501	FAD	O5B-PA-O1A	-2.31	99.80	108.94
2	E	501	FAD	O4'-C4'-C5'	-2.30	104.91	109.99
2	A	501	FAD	C3B-C2B-C1B	2.30	105.81	101.46
2	H	501	FAD	C5A-N7A-C8A	2.29	107.05	103.45
2	A	501	FAD	C4B-O4B-C1B	2.27	114.49	109.47
2	G	501	FAD	O2-C2-N3	2.26	122.92	118.58
2	B	501	FAD	C1'-C2'-C3'	2.25	115.76	109.66
2	E	501	FAD	C4A-C5A-N7A	-2.24	108.02	110.58
2	B	501	FAD	O2-C2-N3	2.23	122.86	118.58
2	C	501	FAD	O2A-PA-O5B	2.23	117.67	107.57
2	A	501	FAD	N6A-C6A-N1A	-2.22	113.43	118.38
2	A	501	FAD	C9A-N10-C10	-2.22	117.36	120.75
2	A	501	FAD	O3'-C3'-C2'	-2.22	103.89	108.93
2	G	501	FAD	C4A-C5A-N7A	-2.21	108.06	110.58
2	E	501	FAD	C4-C4X-N5	2.21	121.25	118.21
2	E	501	FAD	C4A-N9A-C8A	2.20	108.05	105.74
2	F	501	FAD	C10-C4X-N5	-2.19	120.34	124.81
2	D	501	FAD	O2A-PA-O3P	2.18	113.17	107.27
2	F	501	FAD	C4-N3-C2	-2.17	121.79	125.64
2	C	501	FAD	O4-C4-C4X	-2.16	120.82	126.53
2	E	501	FAD	N3-C2-N1	2.16	124.08	119.50
2	F	501	FAD	O5B-PA-O1A	-2.15	100.40	108.94
2	H	501	FAD	N6A-C6A-N1A	2.14	123.15	118.38
2	H	501	FAD	C4A-C5A-N7A	-2.14	108.13	110.58
2	F	501	FAD	C5A-N7A-C8A	2.13	106.80	103.45
2	E	501	FAD	O4B-C1B-N9A	2.12	112.17	108.09
2	D	501	FAD	O2A-PA-O1A	2.12	122.29	112.44
2	F	501	FAD	O2A-PA-O3P	2.11	112.97	107.27
2	B	501	FAD	C5A-N7A-C8A	2.11	106.76	103.45
2	B	501	FAD	O4-C4-C4X	-2.11	120.98	126.53
2	B	501	FAD	C1B-N9A-C8A	2.10	131.76	127.09
2	E	501	FAD	O2A-PA-O1A	2.10	122.21	112.44
2	E	501	FAD	O4'-C4'-C3'	2.09	114.15	109.25
2	D	501	FAD	O2P-P-O1P	2.09	122.18	112.44
2	B	501	FAD	O2P-P-O1P	2.09	122.17	112.44
2	A	501	FAD	O3P-PA-O1A	-2.08	104.45	110.70
2	G	501	FAD	C9A-C5X-N5	-2.08	120.25	122.45
2	E	501	FAD	C4-C4X-C10	2.07	120.48	116.93
2	B	501	FAD	O2'-C2'-C3'	-2.06	104.43	109.25
2	A	501	FAD	C10-C4X-N5	-2.06	120.60	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	FAD	C10-C4X-N5	-2.05	120.63	124.81
2	C	501	FAD	C8M-C8-C9	2.04	123.17	119.57
2	E	501	FAD	O3'-C3'-C4'	2.04	113.57	108.93
2	G	501	FAD	C2B-C3B-C4B	2.03	106.53	102.61
2	E	501	FAD	C6A-C5A-N7A	2.03	136.00	132.09
2	G	501	FAD	C4-N3-C2	-2.02	122.06	125.64
2	H	501	FAD	O2P-P-O1P	2.02	121.83	112.44
2	B	501	FAD	C10-C4X-N5	-2.01	120.70	124.81
2	E	501	FAD	C1'-N10-C9A	2.00	124.53	120.63

There are no chirality outliers.

All (111) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C5B-O5B-PA-O3P
2	A	501	FAD	C2'-C1'-N10-C10
2	A	501	FAD	N10-C1'-C2'-O2'
2	A	501	FAD	N10-C1'-C2'-C3'
2	A	501	FAD	C3'-C4'-C5'-O5'
2	B	501	FAD	C5B-O5B-PA-O1A
2	B	501	FAD	C5B-O5B-PA-O2A
2	B	501	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	C2'-C1'-N10-C10
2	B	501	FAD	N10-C1'-C2'-O2'
2	B	501	FAD	N10-C1'-C2'-C3'
2	B	501	FAD	C2'-C3'-C4'-C5'
2	B	501	FAD	O3'-C3'-C4'-O4'
2	B	501	FAD	O3'-C3'-C4'-C5'
2	B	501	FAD	C3'-C4'-C5'-O5'
2	B	501	FAD	O4'-C4'-C5'-O5'
2	B	501	FAD	C5'-O5'-P-O1P
2	B	501	FAD	C5'-O5'-P-O2P
2	C	501	FAD	C5B-O5B-PA-O2A
2	C	501	FAD	C5B-O5B-PA-O3P
2	C	501	FAD	C2'-C1'-N10-C10
2	C	501	FAD	N10-C1'-C2'-O2'
2	C	501	FAD	N10-C1'-C2'-C3'
2	C	501	FAD	C1'-C2'-C3'-O3'
2	C	501	FAD	C1'-C2'-C3'-C4'
2	C	501	FAD	O2'-C2'-C3'-O3'
2	C	501	FAD	O2'-C2'-C3'-C4'
2	C	501	FAD	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	C	501	FAD	O4'-C4'-C5'-O5'
2	D	501	FAD	C5B-O5B-PA-O1A
2	D	501	FAD	C5B-O5B-PA-O2A
2	D	501	FAD	C2'-C1'-N10-C10
2	D	501	FAD	N10-C1'-C2'-O2'
2	D	501	FAD	C1'-C2'-C3'-C4'
2	D	501	FAD	C3'-C4'-C5'-O5'
2	D	501	FAD	O4'-C4'-C5'-O5'
2	E	501	FAD	N10-C1'-C2'-O2'
2	E	501	FAD	N10-C1'-C2'-C3'
2	E	501	FAD	C3'-C4'-C5'-O5'
2	E	501	FAD	O4'-C4'-C5'-O5'
2	F	501	FAD	C2'-C1'-N10-C10
2	F	501	FAD	N10-C1'-C2'-O2'
2	F	501	FAD	N10-C1'-C2'-C3'
2	F	501	FAD	C2'-C3'-C4'-O4'
2	F	501	FAD	O3'-C3'-C4'-O4'
2	F	501	FAD	C3'-C4'-C5'-O5'
2	F	501	FAD	O4'-C4'-C5'-O5'
2	F	501	FAD	C5'-O5'-P-O2P
2	G	501	FAD	C2'-C1'-N10-C10
2	G	501	FAD	N10-C1'-C2'-O2'
2	G	501	FAD	N10-C1'-C2'-C3'
2	G	501	FAD	C5'-O5'-P-O2P
2	H	501	FAD	C2'-C1'-N10-C9A
2	H	501	FAD	C2'-C1'-N10-C10
2	H	501	FAD	C1'-C2'-C3'-O3'
2	H	501	FAD	C1'-C2'-C3'-C4'
2	H	501	FAD	C3'-C4'-C5'-O5'
2	H	501	FAD	O4'-C4'-C5'-O5'
2	H	501	FAD	C5'-O5'-P-O1P
2	H	501	FAD	C5'-O5'-P-O3P
2	H	501	FAD	O2'-C2'-C3'-O3'
2	B	501	FAD	C2'-C3'-C4'-O4'
2	E	501	FAD	C2'-C3'-C4'-O4'
2	H	501	FAD	O2'-C2'-C3'-C4'
2	F	501	FAD	O3'-C3'-C4'-C5'
2	G	501	FAD	O3'-C3'-C4'-C5'
2	F	501	FAD	C2'-C3'-C4'-C5'
2	G	501	FAD	O3'-C3'-C4'-O4'
2	C	501	FAD	C2'-C3'-C4'-O4'
2	D	501	FAD	O2'-C2'-C3'-C4'

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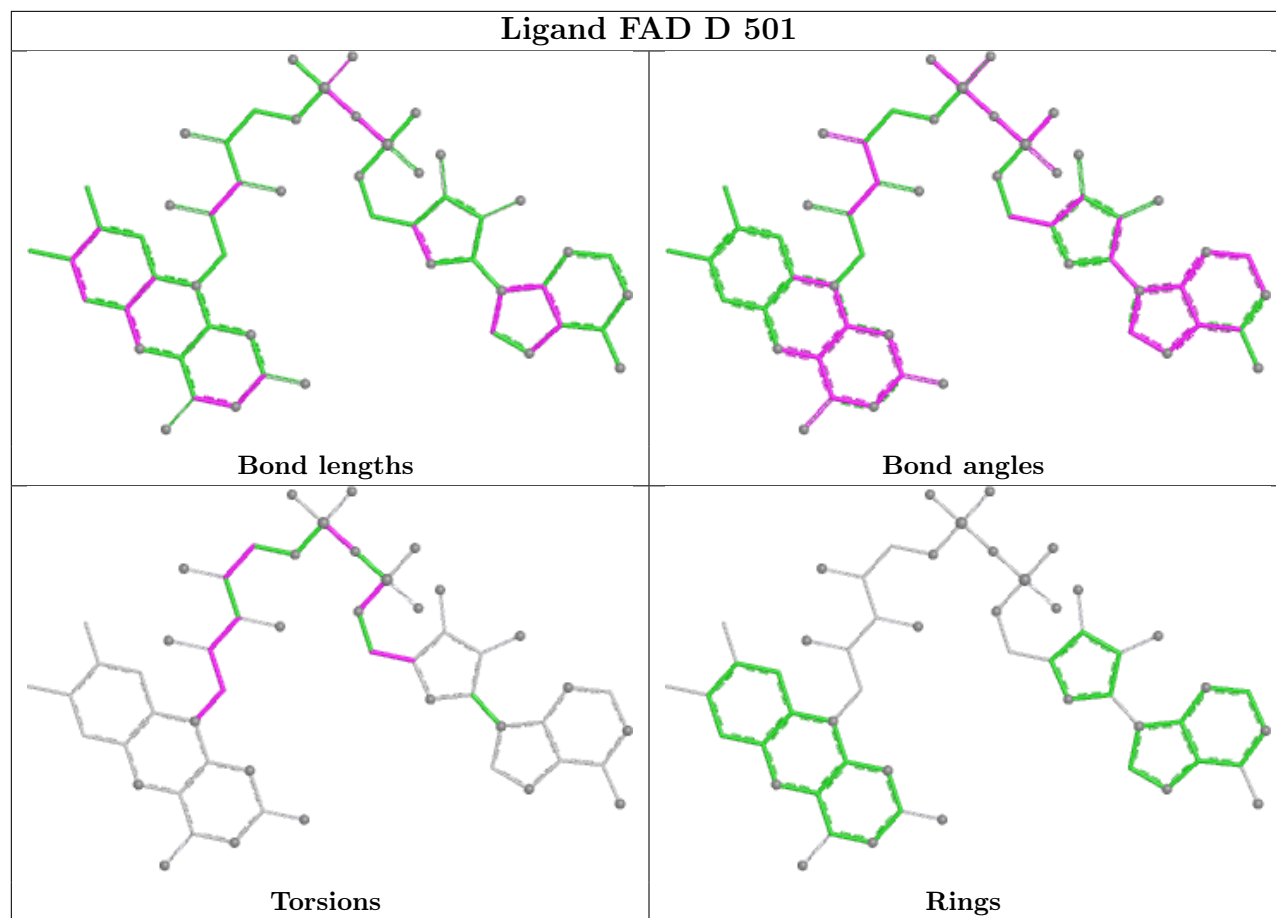
Mol	Chain	Res	Type	Atoms
2	A	501	FAD	O4B-C4B-C5B-O5B
2	A	501	FAD	C3B-C4B-C5B-O5B
2	B	501	FAD	C3B-C4B-C5B-O5B
2	E	501	FAD	O3'-C3'-C4'-C5'
2	E	501	FAD	O3'-C3'-C4'-O4'
2	F	501	FAD	O2'-C2'-C3'-O3'
2	F	501	FAD	O2'-C2'-C3'-C4'
2	G	501	FAD	C2'-C3'-C4'-O4'
2	C	501	FAD	C3B-C4B-C5B-O5B
2	G	501	FAD	C2'-C3'-C4'-C5'
2	C	501	FAD	O3'-C3'-C4'-O4'
2	C	501	FAD	O4B-C4B-C5B-O5B
2	E	501	FAD	C2'-C3'-C4'-C5'
2	E	501	FAD	O4B-C4B-C5B-O5B
2	E	501	FAD	C3B-C4B-C5B-O5B
2	G	501	FAD	P-O3P-PA-O1A
2	C	501	FAD	C2'-C3'-C4'-C5'
2	D	501	FAD	N10-C1'-C2'-C3'
2	D	501	FAD	O2'-C2'-C3'-O3'
2	A	501	FAD	C5B-O5B-PA-O1A
2	A	501	FAD	C5B-O5B-PA-O2A
2	B	501	FAD	C5B-O5B-PA-O3P
2	B	501	FAD	C5'-O5'-P-O3P
2	C	501	FAD	C5B-O5B-PA-O1A
2	C	501	FAD	C5'-O5'-P-O1P
2	C	501	FAD	C5'-O5'-P-O2P
2	C	501	FAD	C5'-O5'-P-O3P
2	D	501	FAD	C5B-O5B-PA-O3P
2	E	501	FAD	C5B-O5B-PA-O1A
2	F	501	FAD	C5'-O5'-P-O1P
2	F	501	FAD	C5'-O5'-P-O3P
2	G	501	FAD	C5'-O5'-P-O1P
2	G	501	FAD	C5'-O5'-P-O3P
2	H	501	FAD	C5'-O5'-P-O2P
2	E	501	FAD	C4'-C5'-O5'-P
2	G	501	FAD	P-O3P-PA-O2A
2	D	501	FAD	C1'-C2'-C3'-O3'
2	C	501	FAD	PA-O3P-P-O1P
2	D	501	FAD	PA-O3P-P-O2P
2	E	501	FAD	P-O3P-PA-O2A
2	D	501	FAD	O4B-C4B-C5B-O5B

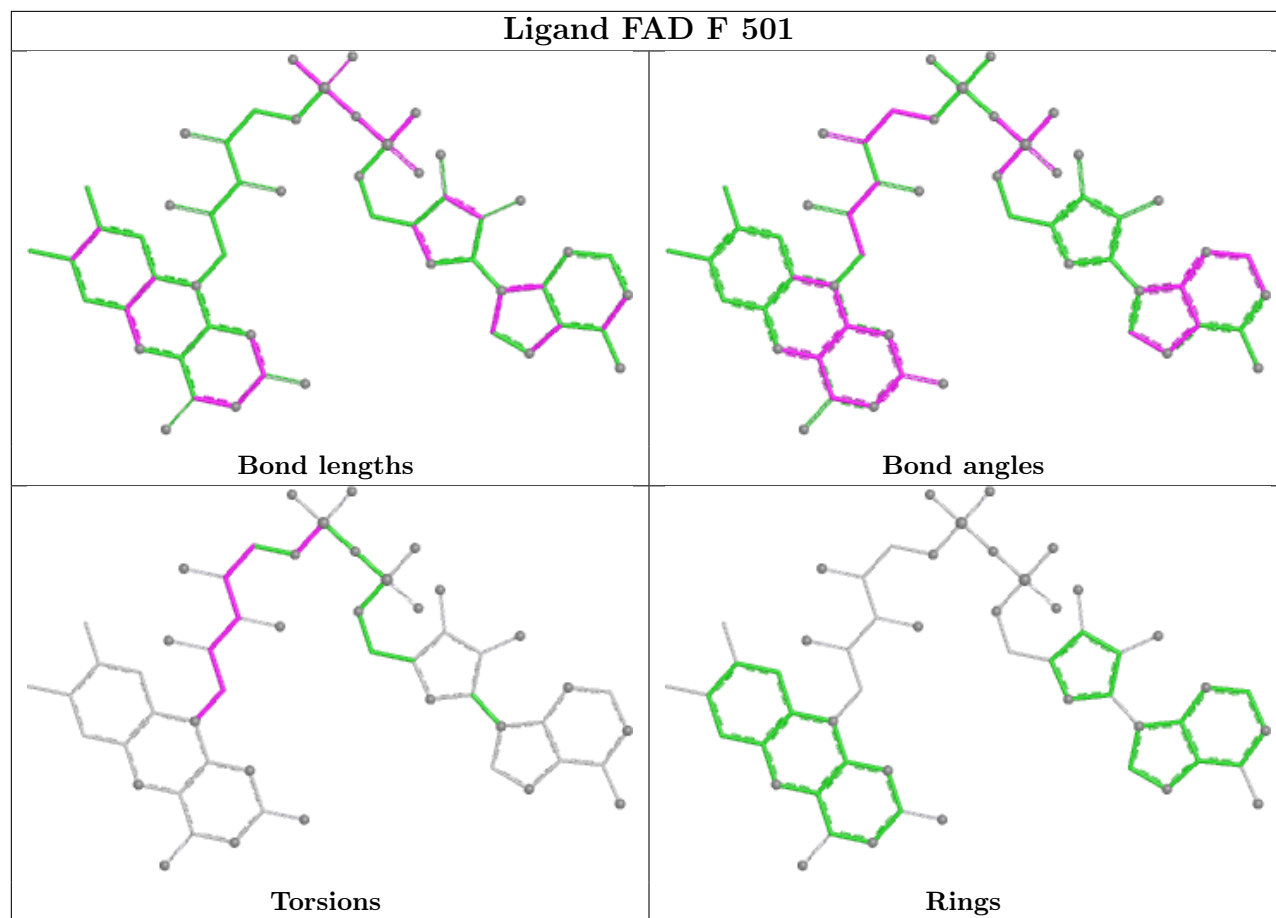
There are no ring outliers.

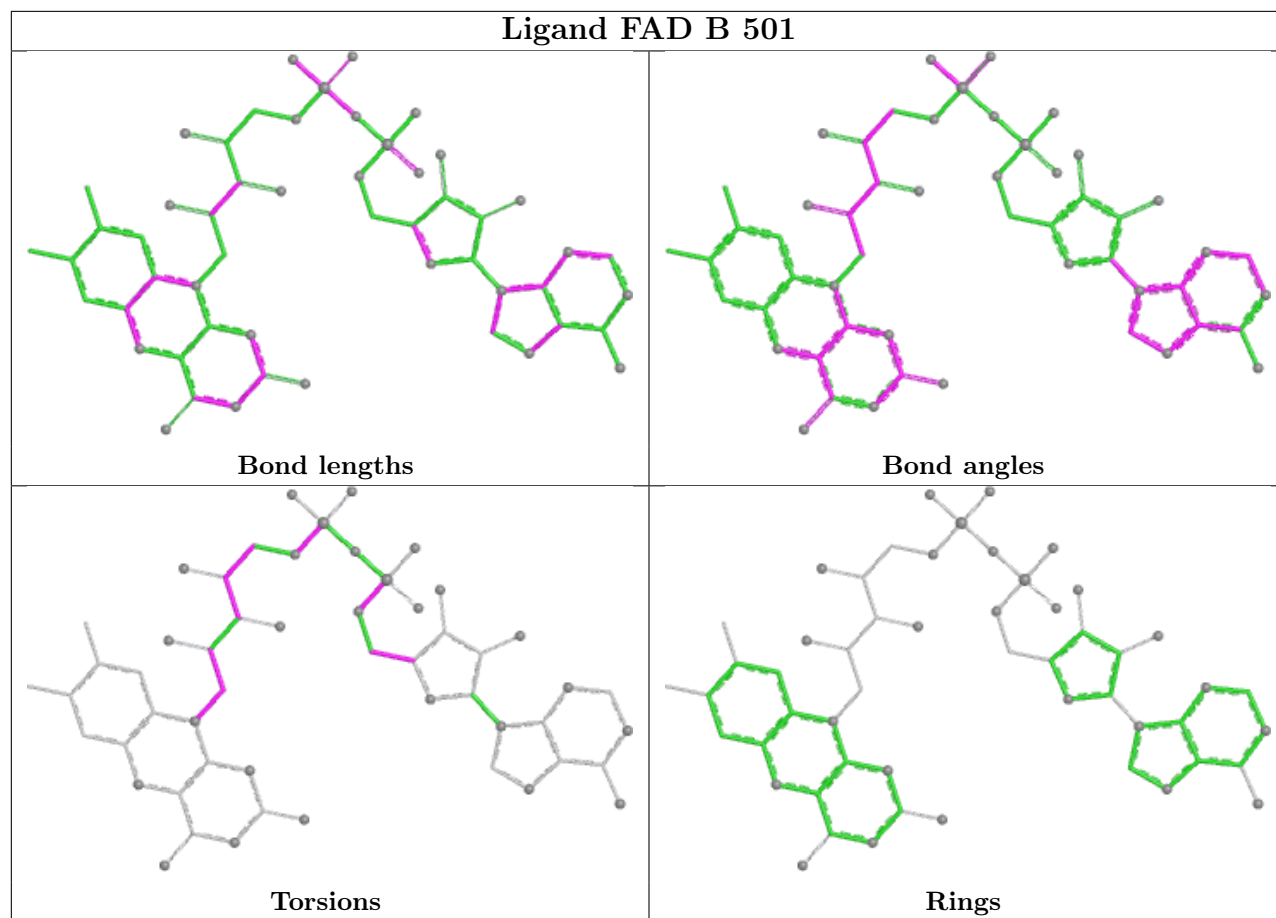
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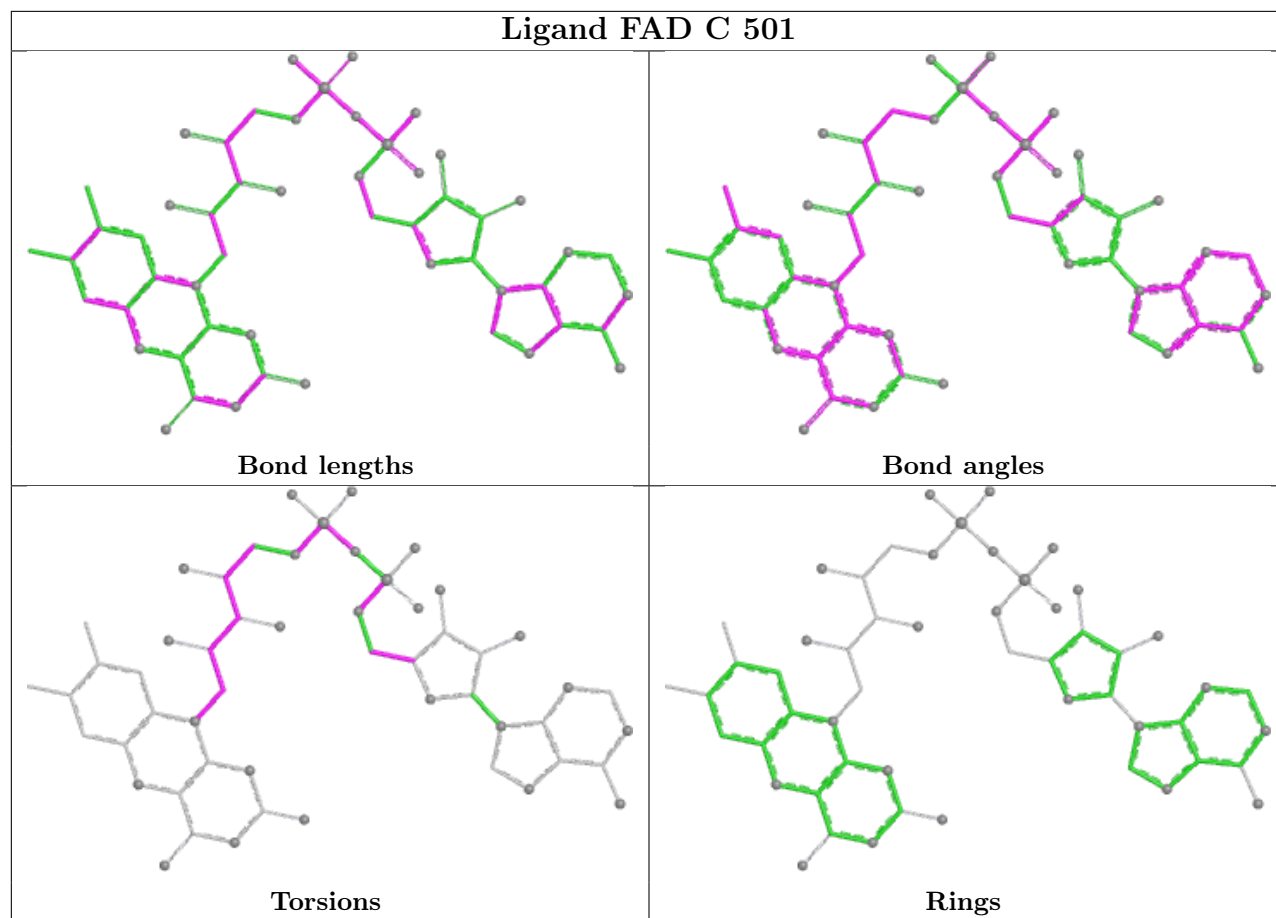
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	FAD	14	0
2	F	501	FAD	18	0
2	B	501	FAD	7	0
2	C	501	FAD	26	0
2	G	501	FAD	11	0
2	A	501	FAD	10	0
2	H	501	FAD	33	0
2	E	501	FAD	30	0

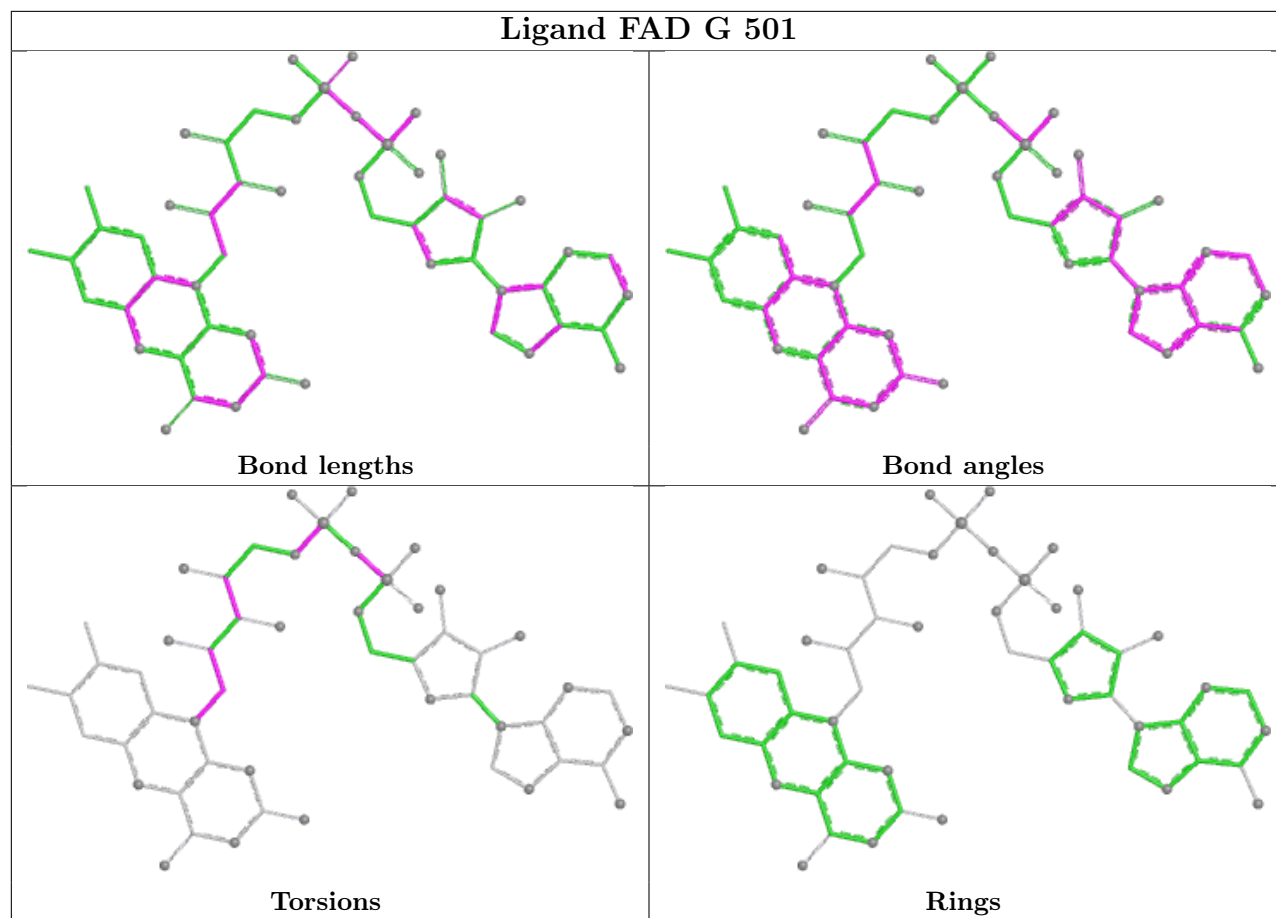
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

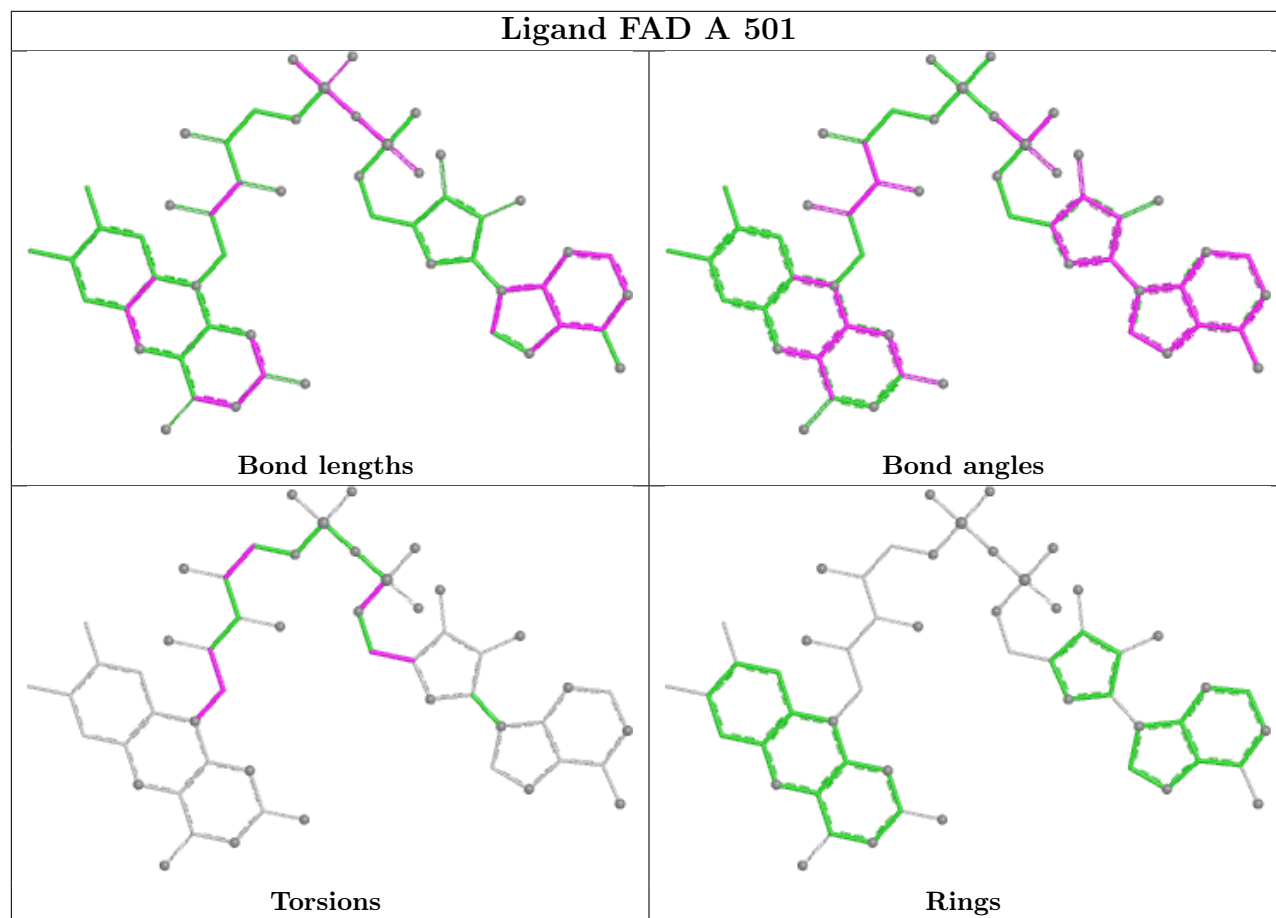


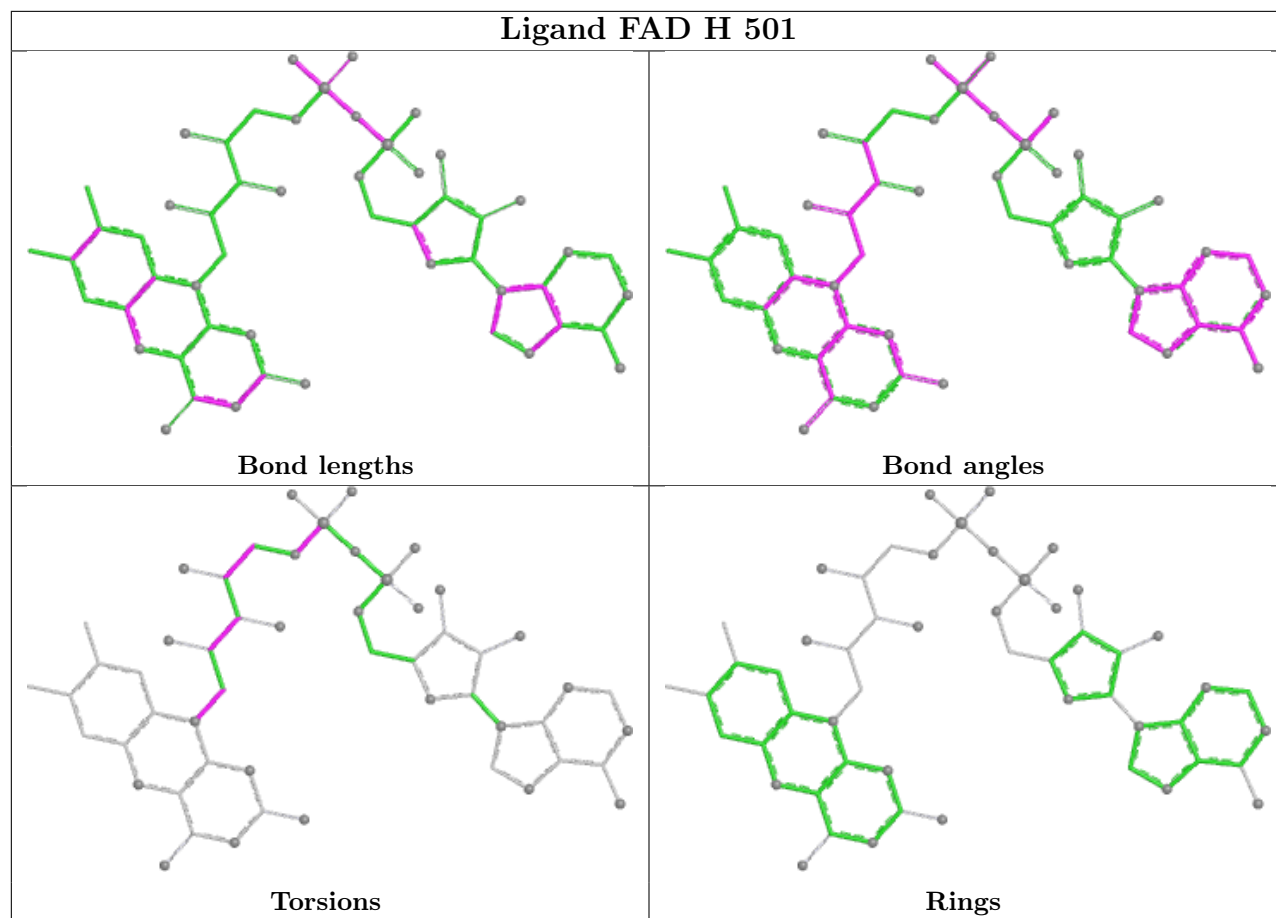


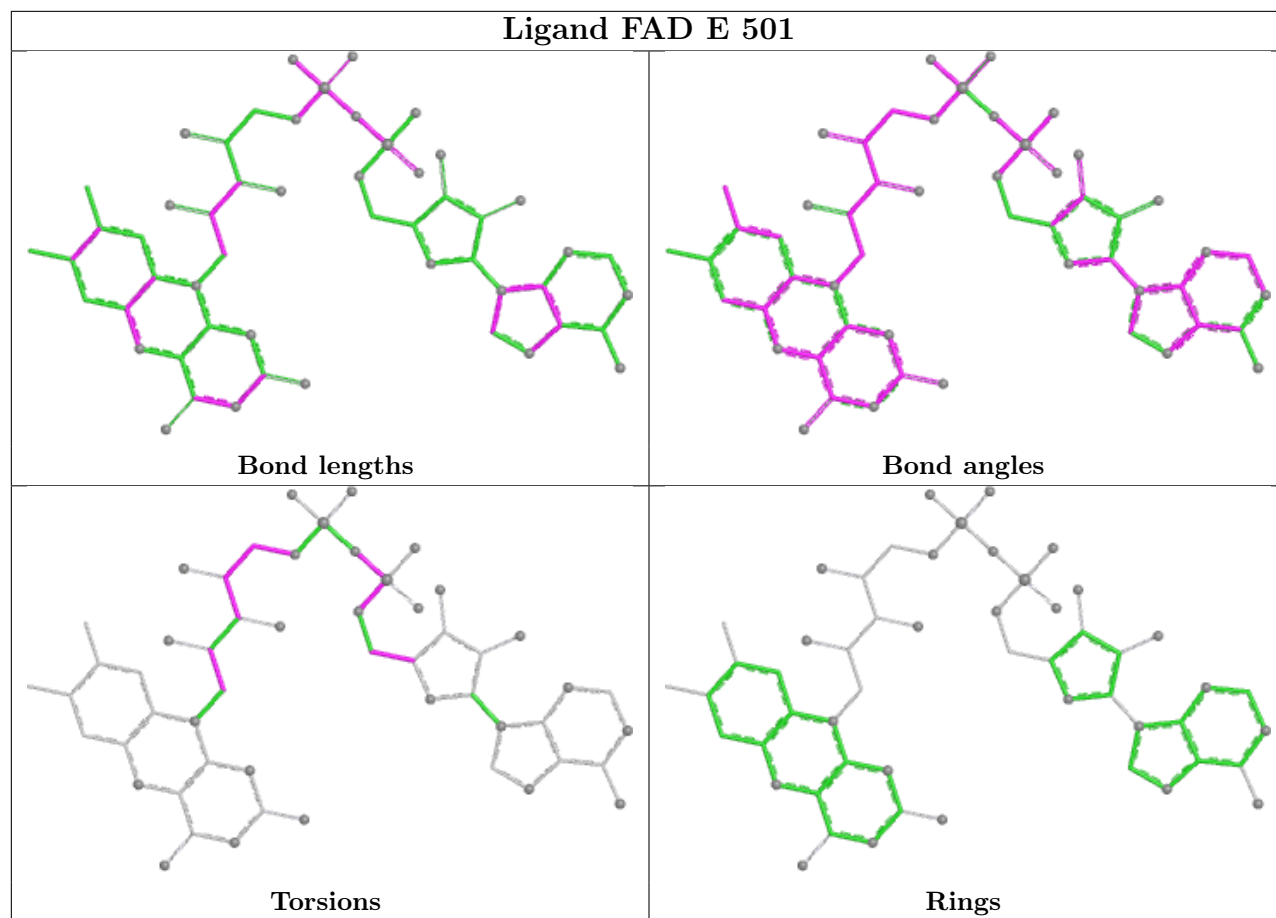












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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 ²)	Q < 0.9
1	A	446/464 (96%)	0.23	16 (3%)	46	37	17, 43, 123, 141	0
1	B	447/464 (96%)	0.23	15 (3%)	48	38	14, 54, 109, 132	0
1	C	445/464 (95%)	0.24	14 (3%)	51	42	19, 53, 117, 166	0
1	D	453/464 (97%)	0.46	26 (5%)	29	22	30, 63, 126, 178	0
1	E	450/464 (96%)	0.49	28 (6%)	26	20	21, 62, 119, 164	0
1	F	444/464 (95%)	0.33	24 (5%)	31	24	14, 56, 130, 191	0
1	G	453/464 (97%)	0.42	20 (4%)	39	30	24, 61, 135, 178	0
1	H	369/464 (79%)	0.36	16 (4%)	40	31	17, 60, 129, 152	0
All	All	3507/3712 (94%)	0.35	159 (4%)	38	30	14, 57, 125, 191	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	233	ALA	12.0
1	C	132	PRO	6.0
1	F	252	LEU	5.5
1	E	322	ALA	5.1
1	A	330	LEU	4.6
1	F	183	ALA	4.6
1	D	257	CYS	4.5
1	G	202	LEU	4.5
1	D	202	LEU	4.4
1	D	457	PHE	4.4
1	E	245	ILE	4.4
1	D	233	ALA	4.3
1	A	295	ILE	4.3
1	D	327	TYR	4.3
1	E	230	LEU	4.2
1	C	295	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	G	116	ASP	3.7
1	A	258	LEU	3.7
1	G	241	SER	3.7
1	D	34	TRP	3.7
1	E	327	TYR	3.7
1	G	245	ILE	3.6
1	H	252	LEU	3.6
1	E	260	ALA	3.5
1	E	232	ASP	3.5
1	H	152	CYS	3.5
1	F	235	ARG	3.5
1	E	231	THR	3.4
1	G	160	ARG	3.3
1	B	327	TYR	3.3
1	H	412	VAL	3.3
1	A	237	VAL	3.3
1	E	275	VAL	3.3
1	C	258	LEU	3.2
1	D	258	LEU	3.2
1	F	257	CYS	3.2
1	B	385	ALA	3.2
1	F	373	GLY	3.2
1	E	298	CYS	3.1
1	H	305	VAL	3.1
1	G	325	LEU	3.1
1	G	298	CYS	3.1
1	H	316	ALA	3.1
1	F	34	TRP	3.1
1	H	426	ALA	3.0
1	F	327	TYR	3.0
1	F	253	ILE	3.0
1	A	252	LEU	3.0
1	E	238	ALA	3.0
1	E	261	VAL	3.0
1	C	299	PHE	3.0
1	F	323	ARG	2.9
1	A	318	ALA	2.9
1	E	156	TYR	2.9
1	B	154	VAL	2.9
1	F	334	GLY	2.8
1	H	328	PRO	2.8
1	G	242	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	8	LEU	2.8
1	D	261	VAL	2.8
1	D	456	VAL	2.8
1	F	35	ALA	2.8
1	A	276	LEU	2.8
1	D	330	LEU	2.7
1	C	364	THR	2.7
1	C	238	ALA	2.7
1	E	115	ASP	2.7
1	H	131	ASP	2.7
1	H	246	VAL	2.7
1	B	375	GLY	2.7
1	D	295	ILE	2.6
1	E	246	VAL	2.6
1	G	204	LEU	2.6
1	G	418	VAL	2.6
1	B	71	ALA	2.6
1	D	214	PRO	2.6
1	F	236	ALA	2.6
1	D	299	PHE	2.5
1	E	291	GLU	2.5
1	D	23	VAL	2.4
1	C	275	VAL	2.4
1	D	90	PHE	2.4
1	D	298	CYS	2.4
1	E	257	CYS	2.4
1	A	38	ASP	2.4
1	H	381	PHE	2.4
1	F	326	ALA	2.4
1	F	458	ALA	2.4
1	G	260	ALA	2.4
1	H	12	ILE	2.4
1	F	328	PRO	2.4
1	D	246	VAL	2.3
1	F	256	PHE	2.3
1	D	286	THR	2.3
1	G	327	TYR	2.3
1	G	295	ILE	2.3
1	D	372	ALA	2.3
1	H	413	THR	2.3
1	F	362	PHE	2.3
1	E	236	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	390	ALA	2.3
1	B	289	GLN	2.3
1	D	369	ILE	2.3
1	E	234	GLY	2.3
1	C	372	ALA	2.2
1	E	292	ALA	2.2
1	D	215	LEU	2.2
1	A	264	TRP	2.2
1	D	284	PRO	2.2
1	B	156	TYR	2.2
1	D	279	ALA	2.2
1	E	239	ALA	2.2
1	A	230	LEU	2.2
1	C	347	ARG	2.2
1	D	4	VAL	2.2
1	F	231	THR	2.2
1	F	156	TYR	2.2
1	D	322	ALA	2.2
1	H	151	LEU	2.2
1	B	115	ASP	2.2
1	G	4	VAL	2.2
1	H	150	GLY	2.2
1	H	306	TYR	2.2
1	B	330	LEU	2.2
1	F	234	GLY	2.2
1	A	305	VAL	2.1
1	A	3	GLY	2.1
1	F	225	GLY	2.1
1	B	256	PHE	2.1
1	F	258	LEU	2.1
1	B	242	ALA	2.1
1	C	346	ALA	2.1
1	C	284	PRO	2.1
1	G	305	VAL	2.1
1	H	308	VAL	2.1
1	C	225	GLY	2.1
1	E	23	VAL	2.1
1	A	328	PRO	2.1
1	B	265	LYS	2.1
1	D	362	PHE	2.1
1	G	398	PHE	2.1
1	G	329	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	153	CYS	2.0
1	C	325	LEU	2.0
1	F	320	PHE	2.0
1	B	364	THR	2.0
1	G	201	THR	2.0
1	C	133	ALA	2.0
1	E	14	ALA	2.0
1	E	228	ASP	2.0
1	E	387	ASP	2.0
1	A	241	SER	2.0
1	A	321	GLN	2.0
1	E	151	LEU	2.0
1	A	347	ARG	2.0
1	E	368	ASN	2.0
1	B	68	GLY	2.0
1	G	264	TRP	2.0
1	E	434	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FE	H	502	1/1	0.80	0.08	97,97,97,97	1
3	FE	D	502	1/1	0.84	0.07	61,61,61,61	1
2	FAD	E	501	53/53	0.87	0.13	36,54,73,77	0
3	FE	A	502	1/1	0.90	0.05	43,43,43,43	1
3	FE	C	502	1/1	0.91	0.11	69,69,69,69	1
2	FAD	H	501	53/53	0.93	0.11	24,49,87,98	0

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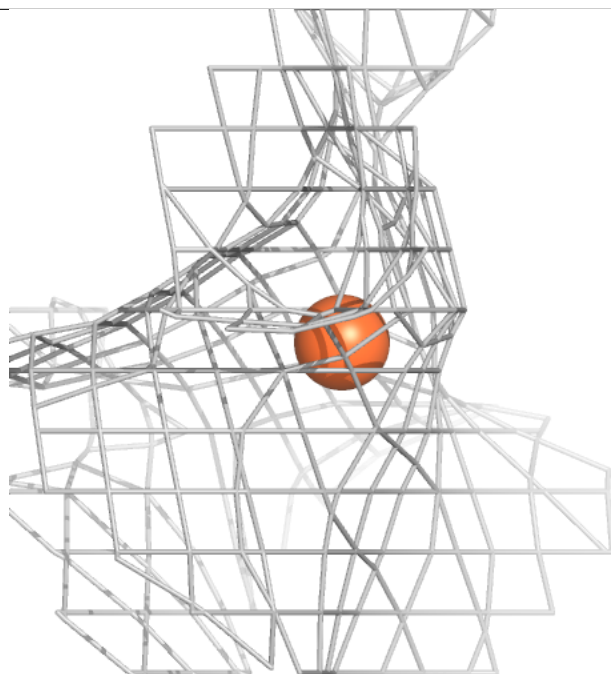
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	C	501	53/53	0.94	0.10	14,40,62,86	0
2	FAD	F	501	53/53	0.94	0.10	19,42,67,90	0
2	FAD	G	501	53/53	0.94	0.08	20,43,61,67	0
2	FAD	D	501	53/53	0.94	0.09	35,52,81,88	0
3	FE	F	502	1/1	0.95	0.12	71,71,71,71	1
2	FAD	A	501	53/53	0.95	0.09	17,39,60,74	0
2	FAD	B	501	53/53	0.96	0.07	17,36,49,55	0
3	FE	B	502	1/1	0.97	0.04	56,56,56,56	1
3	FE	G	502	1/1	0.97	0.04	57,57,57,57	1
3	FE	E	502	1/1	0.97	0.04	59,59,59,59	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

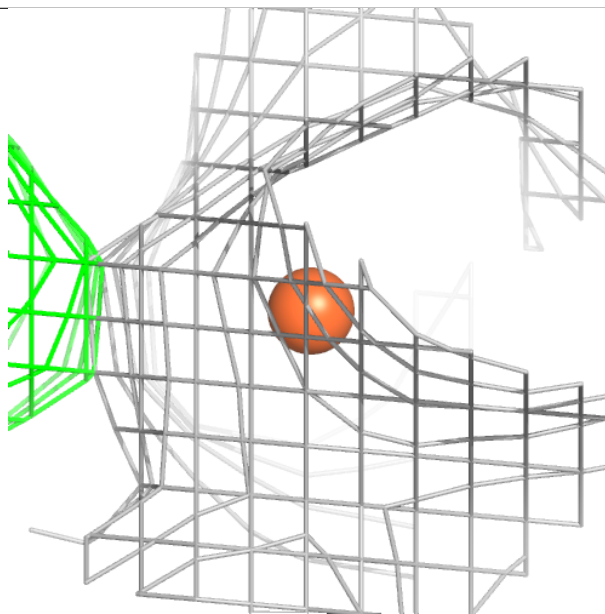
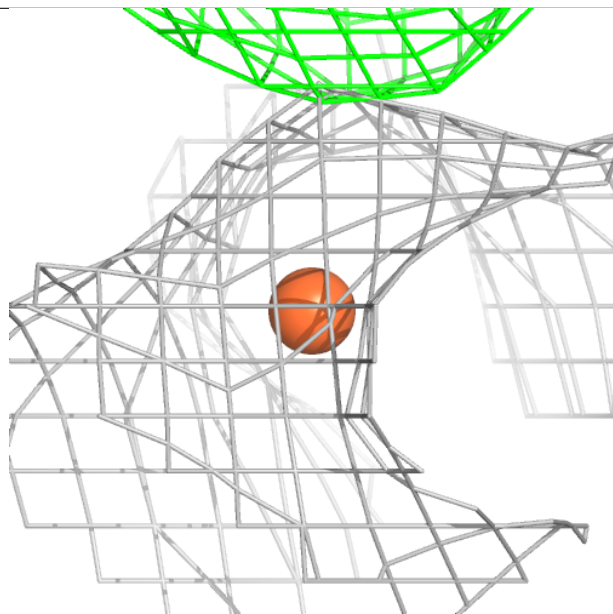
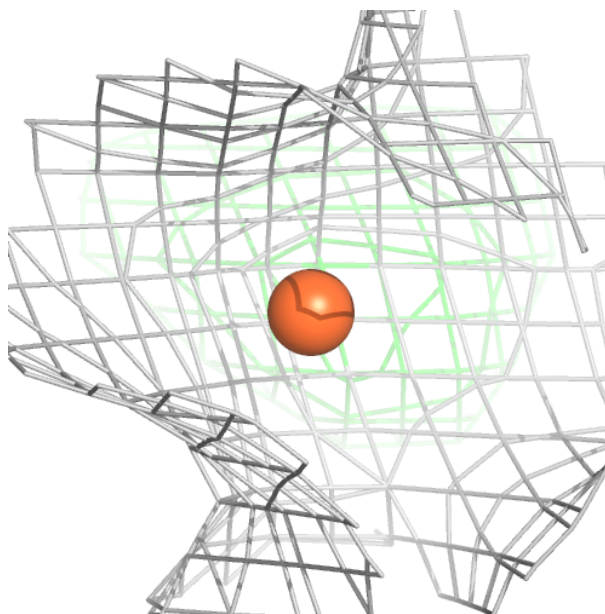
Electron density around FE H 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



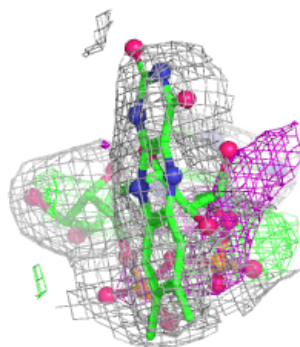
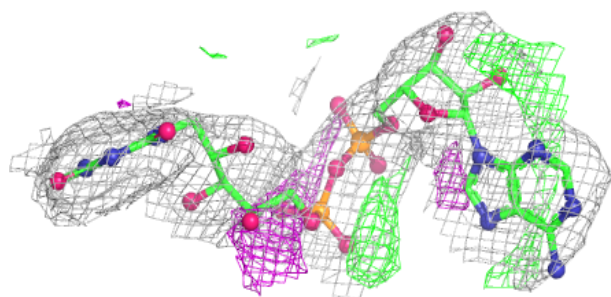
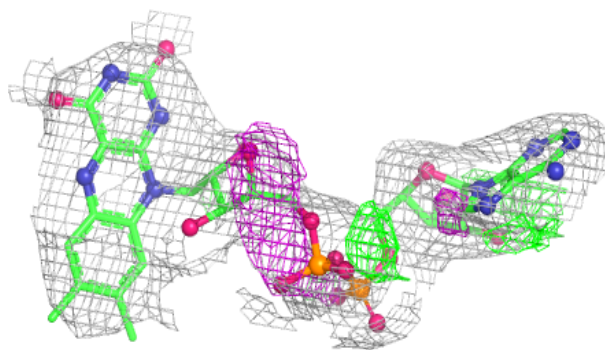
Electron density around FE D 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



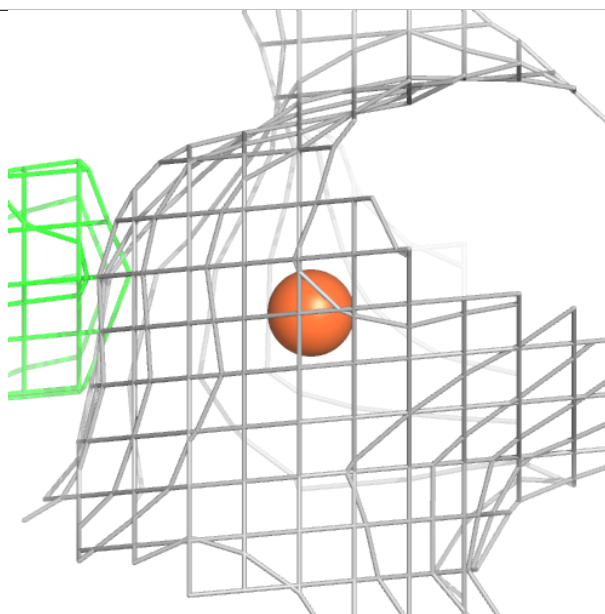
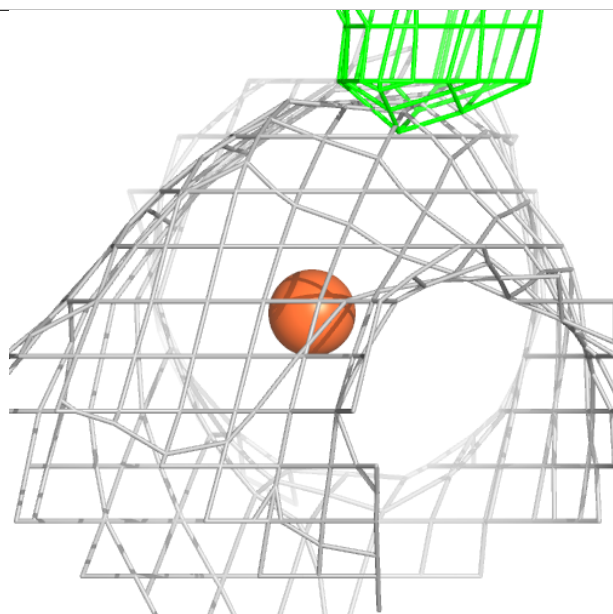
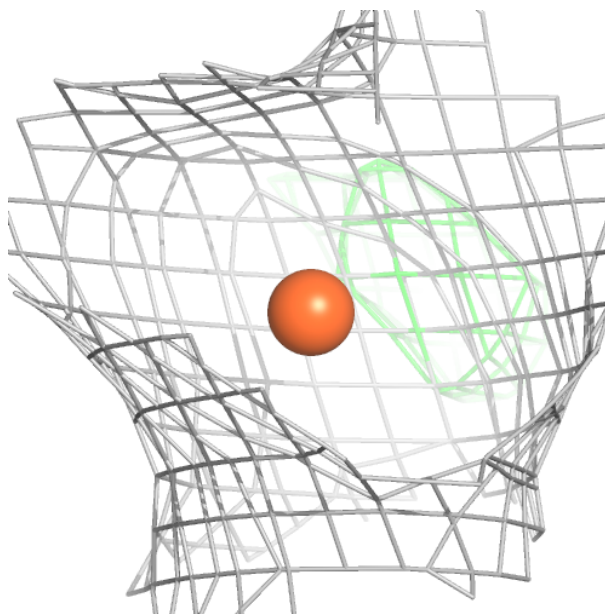
Electron density around FAD E 501:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



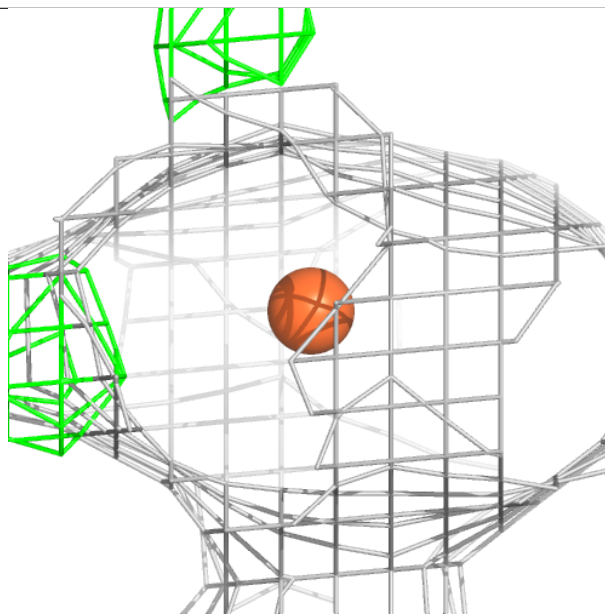
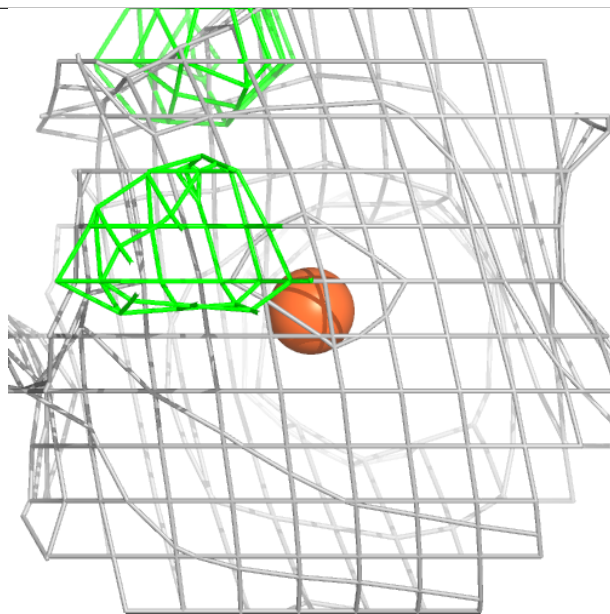
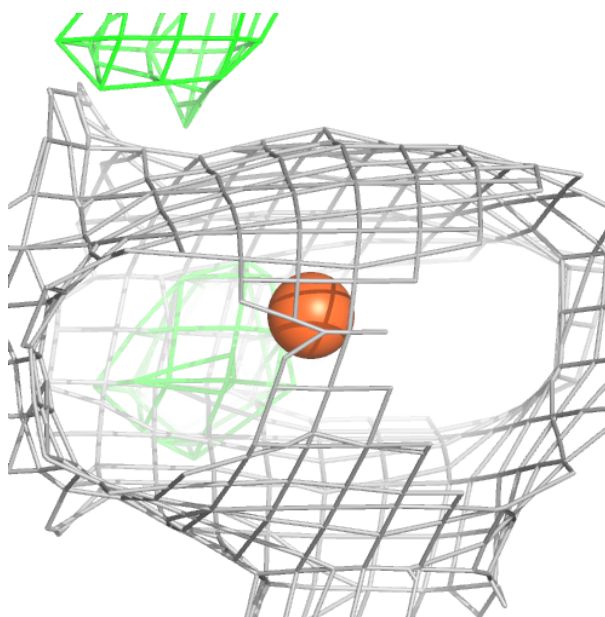
Electron density around FE A 502:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



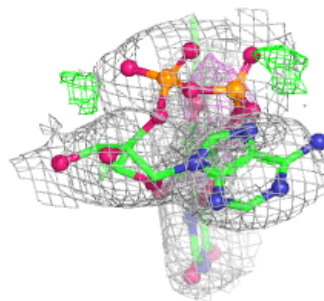
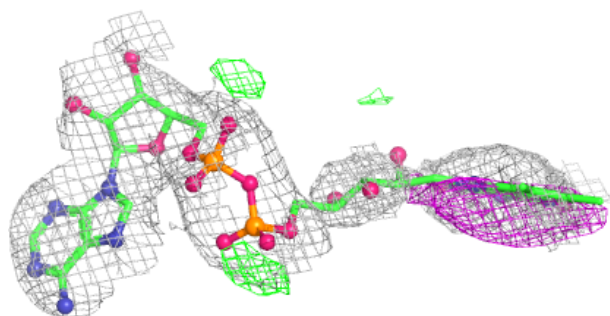
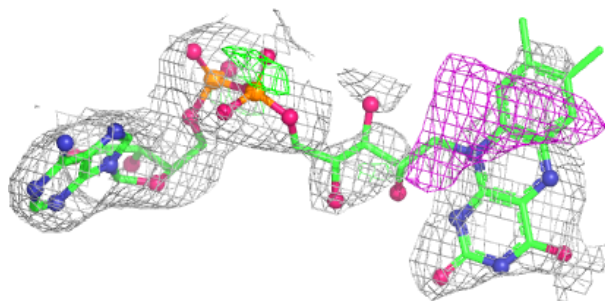
Electron density around FE C 502:

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and green (positive)

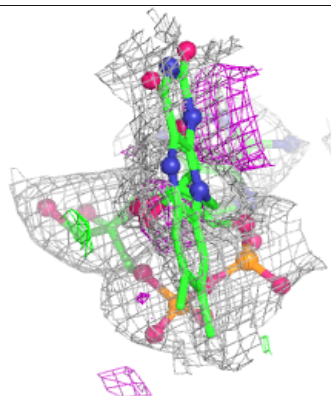
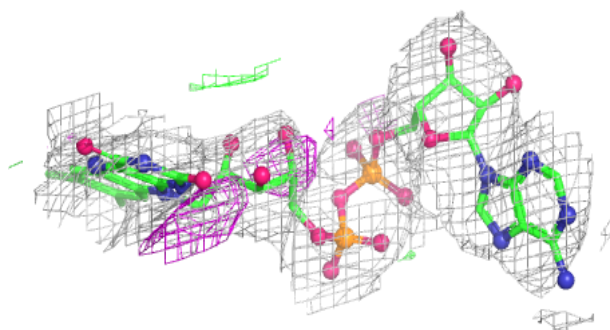
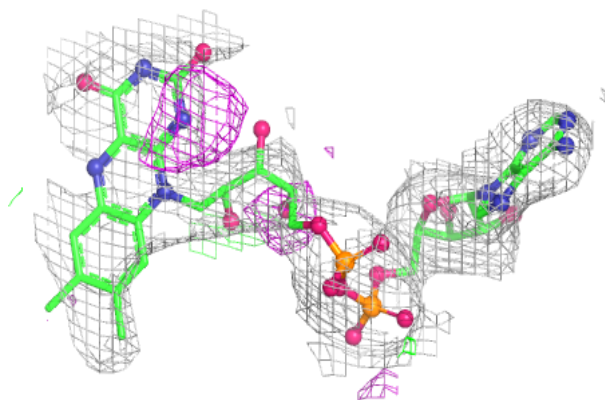


Electron density around FAD H 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

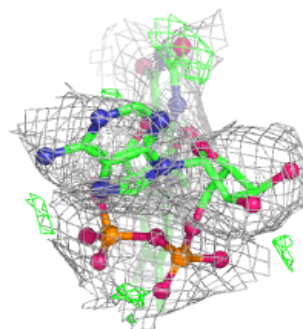
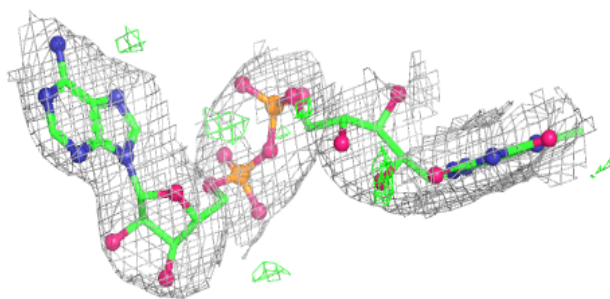
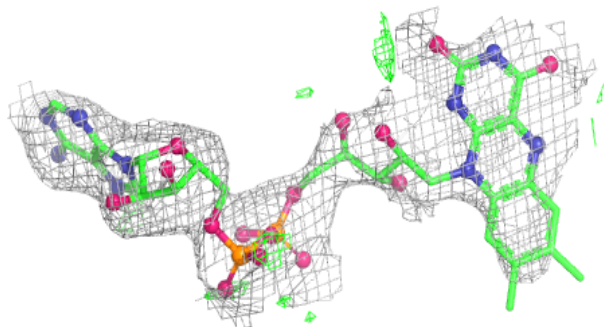
**Electron density around FAD C 501:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

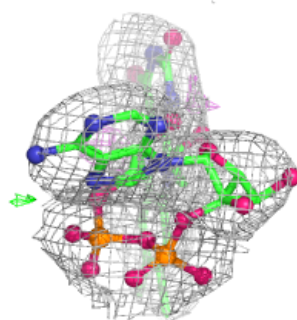
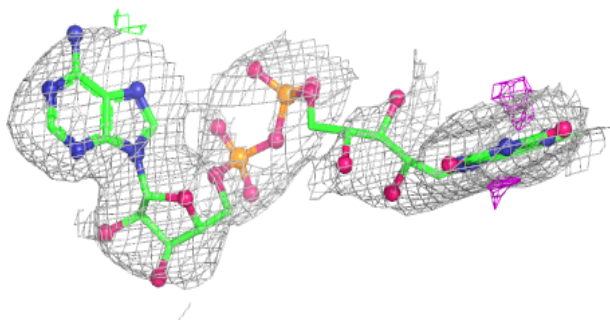
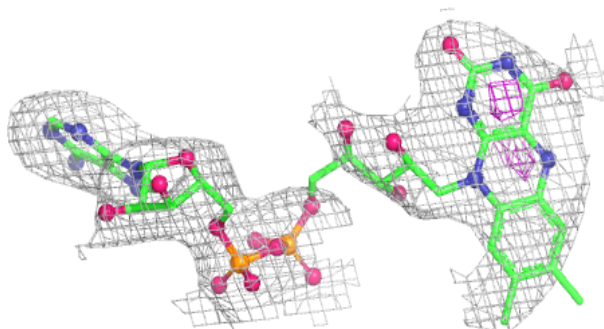


Electron density around FAD F 501:

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 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

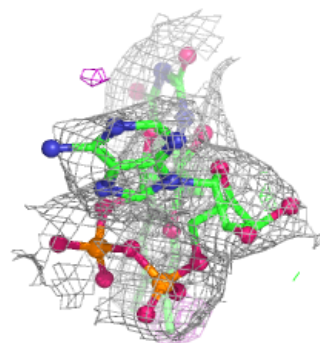
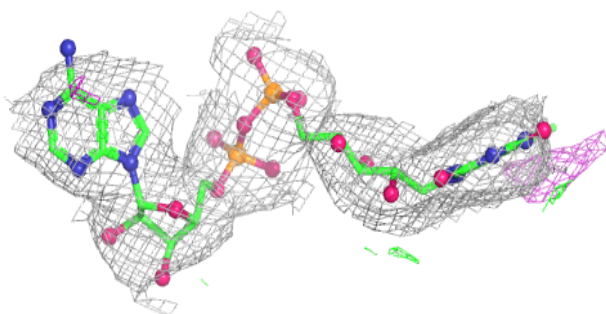
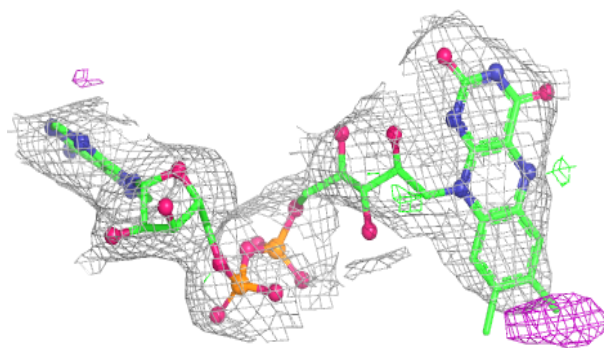
**Electron density around FAD G 501:**

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 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



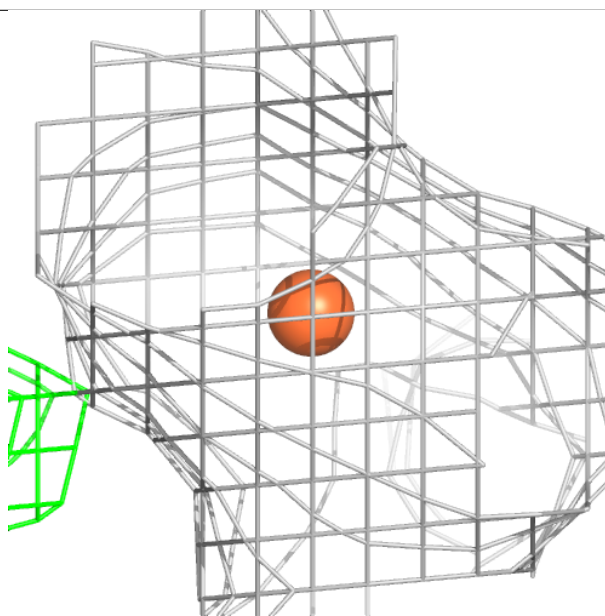
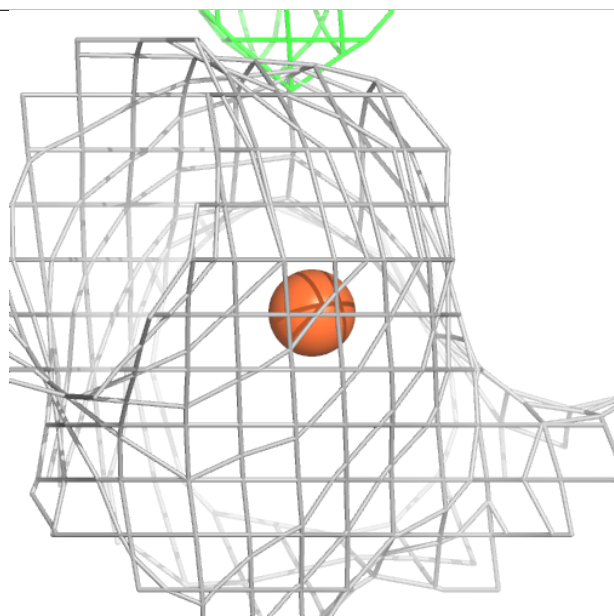
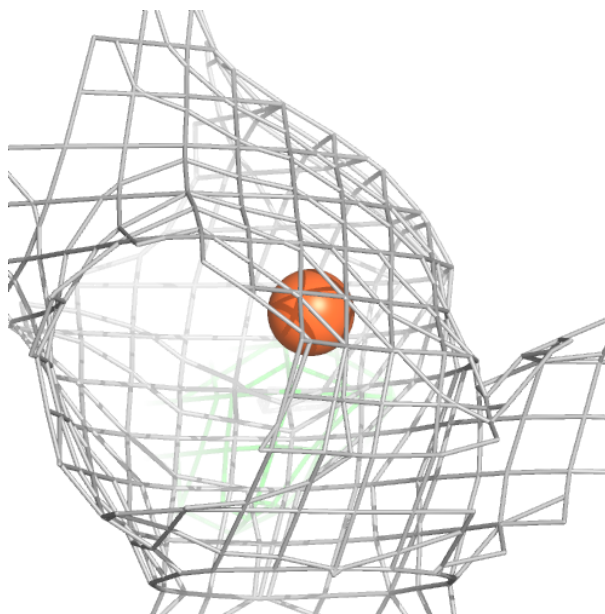
Electron density around FAD D 501:

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and green (positive)



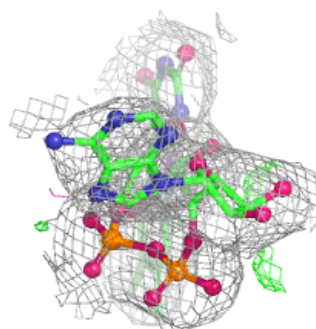
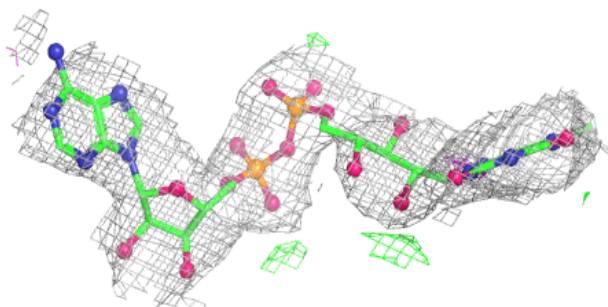
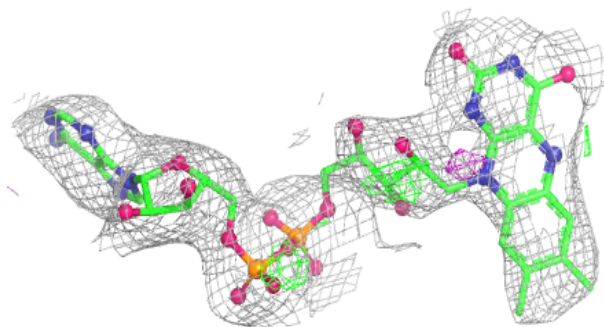
Electron density around FE F 502:

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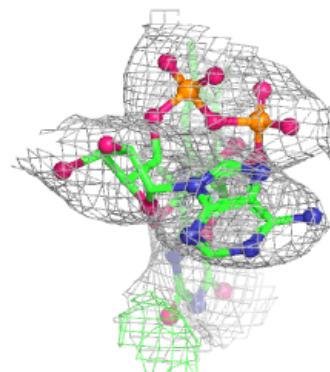
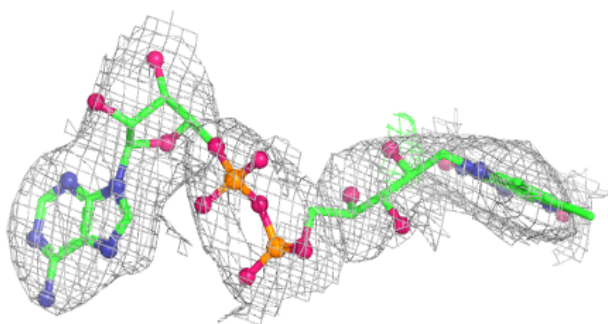
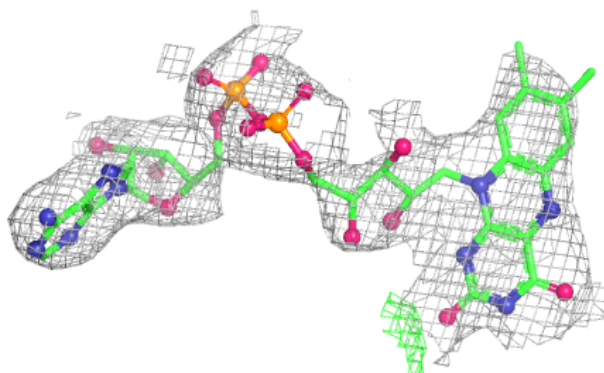


Electron density around FAD A 501:

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and green (positive)

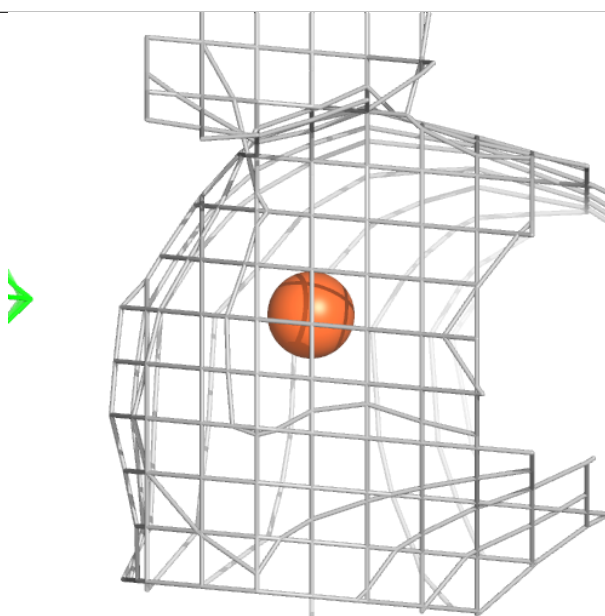
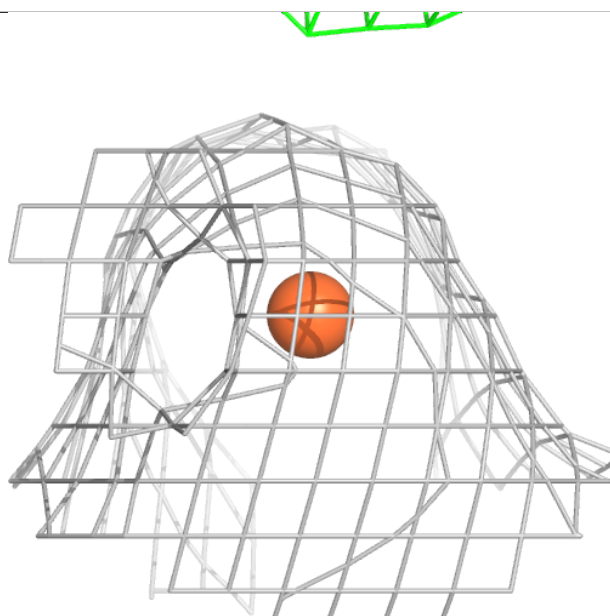
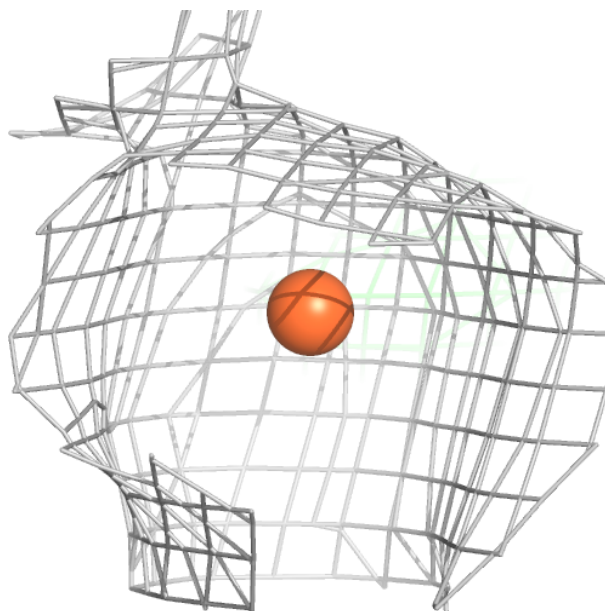
**Electron density around FAD B 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



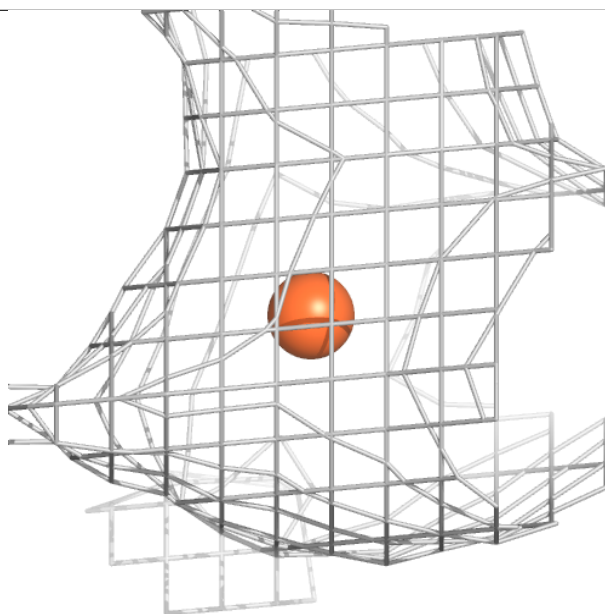
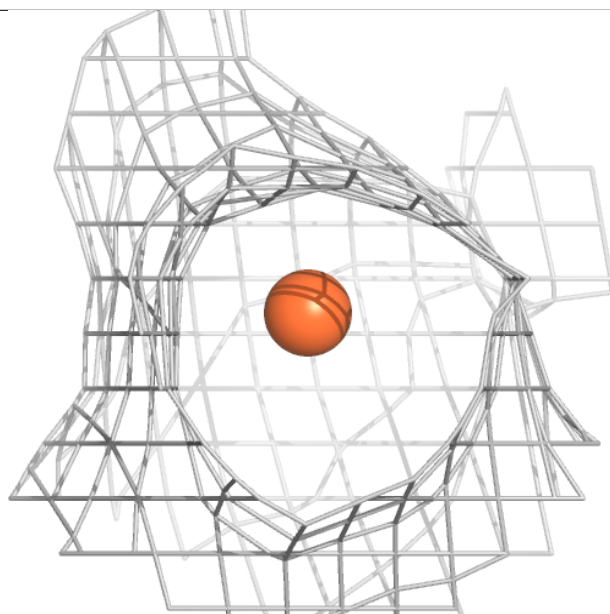
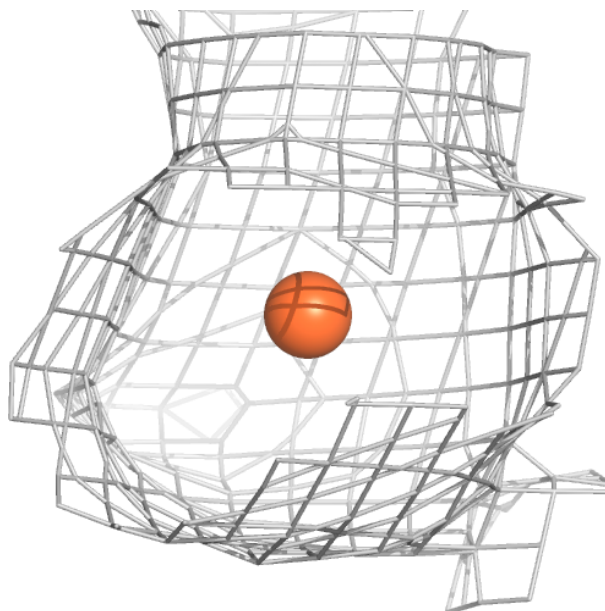
Electron density around FE B 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE G 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.