



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 11, 2022 – 07:17 pm BST

PDB ID : 7QFX  
Title : Crystal structure of Old Yellow Enzyme AnOYE8 from *Aspergillus niger*  
Authors : Robescu, M.S.; Loprete, G.; Vascon, F.; Gasparotto, M.; Filippini, F.;  
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Deposited on : 2021-12-06  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

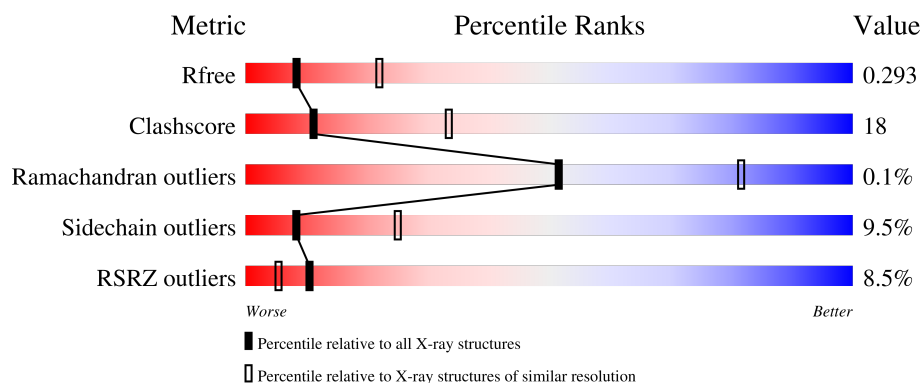
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	B	422	<div> <div>3%</div> <div>59%</div> <div>31%</div> <div>6%</div> <div>.</div> </div>
1	C	422	<div> <div>3%</div> <div>66%</div> <div>29%</div> <div>.</div> <div>.</div> </div>
1	E	422	<div> <div>11%</div> <div>60%</div> <div>33%</div> <div>.</div> <div>.</div> </div>
1	G	422	<div> <div>15%</div> <div>59%</div> <div>31%</div> <div>6%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MPD	E	501	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12791 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 NADH-dependent flavin oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	407	Total	C	N	O	S	0	0	0
			3123	1985	556	573	9			
1	C	413	Total	C	N	O	S	0	0	0
			3167	2010	563	585	9			
1	E	409	Total	C	N	O	S	0	0	0
			3143	1995	561	578	9			
1	G	407	Total	C	N	O	S	0	0	0
			3121	1983	551	578	9			

There are 4 discrepancies between the modelled and reference sequences:

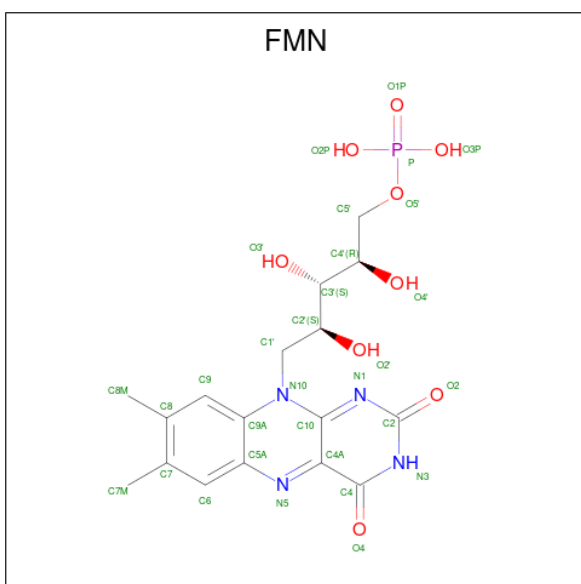
Chain	Residue	Modelled	Actual	Comment	Reference
B	422	PRO	-	expression tag	UNP A0A370CG11
C	427	PRO	-	expression tag	UNP A0A370CG11
E	422	PRO	-	expression tag	UNP A0A370CG11
G	422	PRO	-	expression tag	UNP A0A370CG11

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



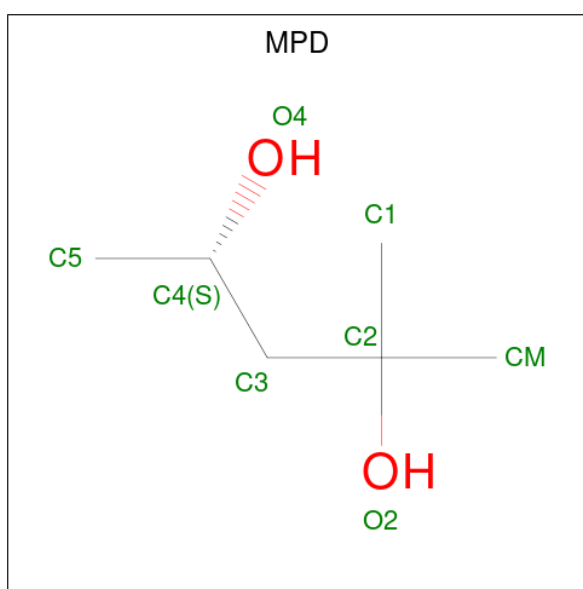
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			8	6	2		

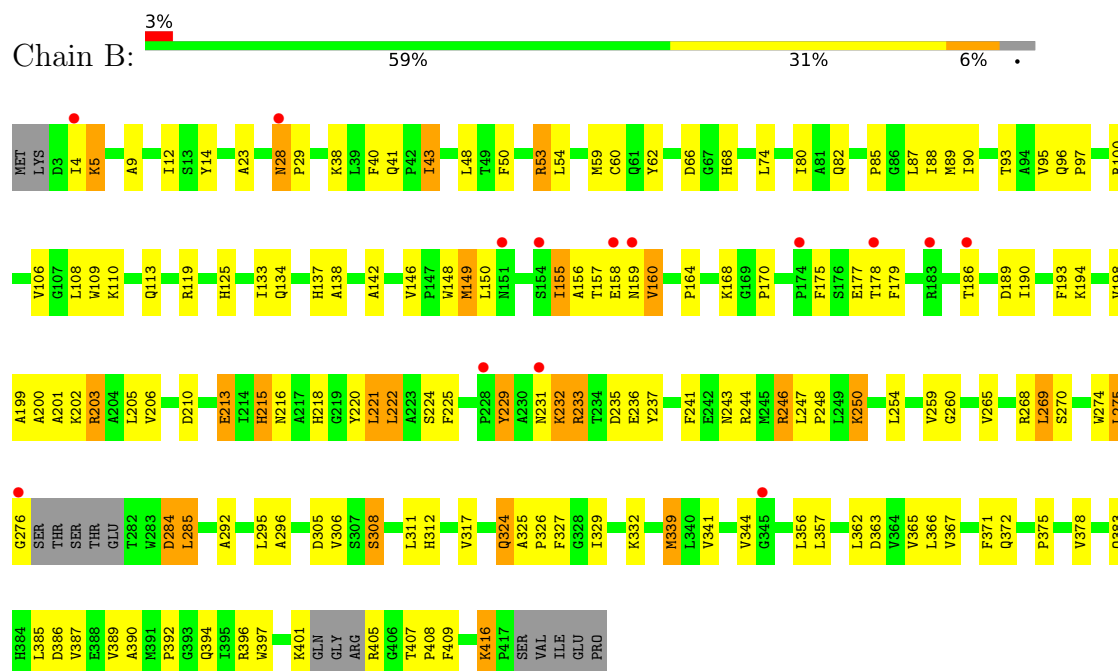
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	20	Total	O	0	0
			20	20		
5	C	41	Total	O	0	0
			41	41		
5	E	14	Total	O	0	0
			14	14		
5	G	10	Total	O	0	0
			10	10		

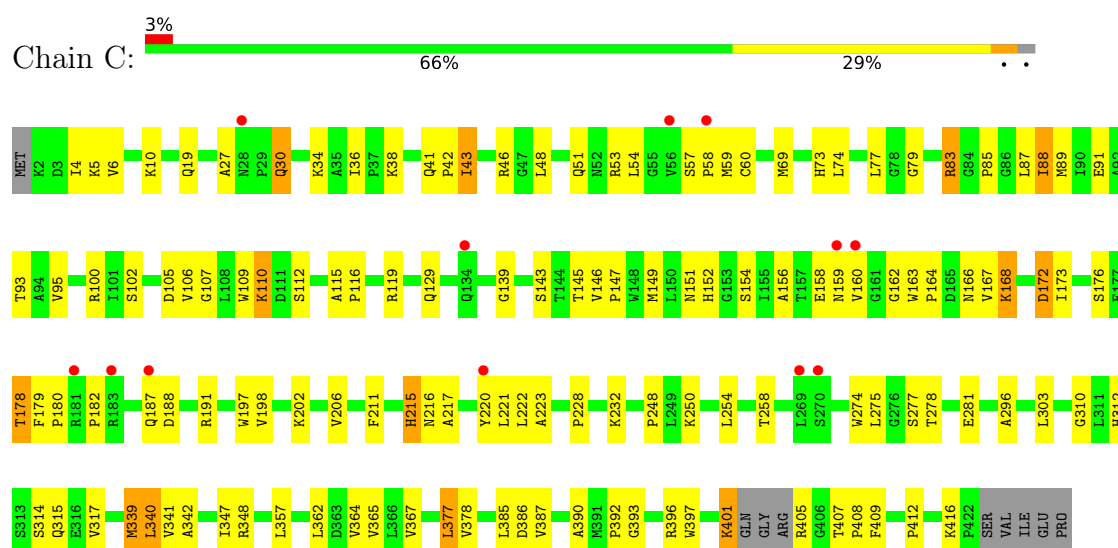
### 3 Residue-property plots

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: NADH-dependent flavin oxidoreductase



- Molecule 1: NADH-dependent flavin oxidoreductase



Chain E:

11% 60% 33%

Chain E: MET LYS D3 I4 E7 P8 I12 T21 P22 A23 A27 N28 P29 Q30 K34 A35 K38 L39 F40 Q41 P42 I43 R46 Q51 N52 R53 S57 P58 M59 C60 Q61 Y62 D71 L74 R83 P85 G86 R87 I88 T83 Q96 V106 V100

Chain G:

15% 59% 31% 6%

MET D3 I4 K5 I12 T16 A27 N28 P29 Q30 T31 S32 G33 K34 K38 I43 T44 I45 G47 L48 T49 F50 Q51 N52 R53 P58 M59 Y62 G67 H68 M69 L74 G79 R83 G84 P85 G86 L87 I88 M89 I90 P97 E98 G99 I100 L101 S102 D105 V106 L108 M109 K110 D111 I114 A115 I117 H125 Q129 K130 I131 G132 I133 Q134 I135 A136 I137 A138 A142 V146 P147 M148 L149 L150 M151 I155 V160 V167 K168 G169 P170 S171 D172 I173 E177 T178 L179 P180 I181 P182 R183 A184 M185 T186 G187 S188 D189 I190 E191 R192 F193 K194 W197 V198 A199 R202 R203 A204 L205 V206 K209 D210 F211 I212 E213 T214 H215 N216 A217 H218 G219 V220 Y221 S224 F225 L226 T227 F228 Y229 A230 A231 K232 ARG T234 D235 E236 S240 F241 E242 N243 R244 K245 R246 L247 P248 L249 K250 T251 L254 T255 T258 V259 H262 F266 S270 A271 W274 L275 GLY SER THR S279 T280 E281 T282 V283 D284 L285 Q286 H287 A288 V289 R290 F291 A294 L295 L303 L307 ARG A308 L311 H312 S313 V317 Q324 A325 P326 K332 V335 G336 E337 R338 M339 T340 V341 A342 T343 V344 I347 R348 D349 G350 K351 R355 L356 L357 E358 E359 E360 G361 L362 R369 K373 W379 E388 R389 A390 Q394 F399 S400 K401 K402 G406 A408 T407 P408 D411 P412 S413 P414 V414 Y415 K416 PRO SER SER VAL ILE GLU PRO



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.53Å 65.39Å 181.42Å 90.00° 107.76° 90.00°	Depositor
Resolution (Å)	39.95 – 2.80 39.95 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (39.95-2.80) 90.0 (39.95-2.80)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, $R_{free}$	0.241 , 0.266 0.269 , 0.293	Depositor DCC
$R_{free}$ test set	1942 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	12791	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MPD, SO4, FMN

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	B	0.58	0/3201	0.69	1/4345 (0.0%)
1	C	0.58	0/3246	0.76	0/4407
1	E	0.55	0/3220	0.75	3/4369 (0.1%)
1	G	0.59	0/3197	0.75	4/4339 (0.1%)
All	All	0.57	0/12864	0.74	8/17460 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	43	ILE	CG1-CB-CG2	5.88	124.35	111.40
1	G	355	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	B	5	LYS	CD-CE-NZ	-5.63	98.76	111.70
1	G	108	LEU	CB-CG-CD2	-5.59	101.49	111.00
1	E	352	LEU	CB-CG-CD2	5.58	120.49	111.00
1	E	416	LYS	CD-CE-NZ	5.48	124.30	111.70
1	G	105	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	E	396	ARG	NE-CZ-NH2	-5.16	117.72	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3123	0	3089	120	0
1	C	3167	0	3133	96	0
1	E	3143	0	3108	129	0
1	G	3121	0	3078	124	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	E	5	0	0	0	0
2	G	5	0	0	0	0
3	B	31	0	19	5	0
3	C	31	0	19	7	0
3	E	31	0	19	4	0
3	G	31	0	19	7	0
4	E	8	0	14	6	0
5	B	20	0	0	1	0
5	C	41	0	0	0	0
5	E	14	0	0	0	0
5	G	10	0	0	1	0
All	All	12791	0	12498	451	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (451) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LEU:HD13	1:B:222:LEU:H	1.20	1.04
1:B:260:GLY:HA3	4:E:501:MPD:H11	1.40	1.00
1:C:312:HIS:HD2	1:C:314:SER:H	1.08	0.96
1:E:71:ASP:HB3	1:G:74:LEU:HD21	1.49	0.95
1:E:21:THR:HG21	1:E:408:PRO:HG3	1.55	0.87
1:E:310:GLY:H	1:E:315:GLN:HE22	1.22	0.85
1:E:231:ASN:HD21	1:E:238:GLY:HA2	1.41	0.84
1:E:168:LYS:HG2	1:E:183:ARG:HE	1.42	0.83
1:C:146:VAL:HG13	1:C:149:MET:HG3	1.60	0.83
1:B:134:GLN:HG3	1:B:213:GLU:HG2	1.60	0.83
1:B:9:ALA:HB3	1:B:12:ILE:HD13	1.60	0.82
1:C:312:HIS:O	1:C:315:GLN:HG2	1.81	0.81
1:E:262:HIS:CD2	4:E:501:MPD:H12	2.16	0.80
1:B:221:LEU:HD13	1:B:222:LEU:N	1.97	0.80
1:E:262:HIS:HD2	4:E:501:MPD:H12	1.44	0.79
1:E:146:VAL:HG13	1:E:149:MET:HG3	1.66	0.76
1:E:166:ASN:HA	1:E:183:ARG:HH22	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:ILE:HD11	1:E:232:LYS:HD2	1.69	0.75
1:E:243:ASN:O	1:E:246:ARG:HB2	1.87	0.74
1:G:59:MET:HA	3:G:501:FMN:N5	2.03	0.73
1:C:310:GLY:N	1:C:315:GLN:HE22	1.86	0.73
1:C:310:GLY:H	1:C:315:GLN:HE22	1.36	0.72
1:C:85:PRO:HG2	1:C:88:ILE:HD13	1.70	0.72
1:G:43:ILE:HG23	1:G:53:ARG:NH2	2.04	0.72
1:G:100:ARG:HG2	1:G:105:ASP:HB2	1.71	0.72
1:B:274:TRP:HE1	1:B:308:SER:HB3	1.55	0.71
1:B:237:TYR:CD2	1:B:246:ARG:HD3	2.28	0.69
1:G:114:ILE:HD11	1:G:203:ARG:HB2	1.75	0.69
1:E:312:HIS:O	1:E:315:GLN:HG2	1.92	0.69
1:C:312:HIS:CD2	1:C:314:SER:H	2.00	0.69
1:E:149:MET:HB3	1:G:4:ILE:HD11	1.75	0.69
1:B:155:ILE:HD11	1:B:164:PRO:HB3	1.76	0.68
1:G:90:ILE:HD12	1:G:133:ILE:HG12	1.75	0.68
1:C:51:GLN:HE22	1:C:129:GLN:HE22	1.42	0.68
1:G:90:ILE:HG13	1:G:131:ILE:HD11	1.76	0.68
1:B:409:PHE:HE2	1:E:29:PRO:HG3	1.59	0.67
1:C:408:PRO:HG2	1:C:409:PHE:CE2	2.30	0.67
1:E:43:ILE:HD11	1:E:53:ARG:HG2	1.77	0.67
1:G:329:ILE:HG12	1:G:360:GLU:HB3	1.77	0.67
1:B:93:THR:HG23	1:B:106:VAL:HG12	1.77	0.66
1:B:138:ALA:HB3	1:B:142:ALA:HB2	1.77	0.66
1:C:172:ASP:OD1	1:C:172:ASP:O	2.13	0.66
1:B:95:VAL:HG23	1:B:96:GLN:HG3	1.78	0.65
1:B:390:ALA:HA	1:B:408:PRO:O	1.97	0.65
1:E:93:THR:HG23	1:E:106:VAL:HG12	1.79	0.65
1:B:53:ARG:HG2	1:B:363:ASP:O	1.97	0.65
1:B:43:ILE:HD12	1:B:50:PHE:HB2	1.79	0.65
1:E:273:ASP:HB3	1:E:311:LEU:HD12	1.80	0.64
1:C:146:VAL:HG13	1:C:149:MET:CG	2.27	0.64
1:B:108:LEU:O	1:B:203:ARG:HD2	1.97	0.64
1:B:137:HIS:HB3	1:B:221:LEU:CD1	2.28	0.64
1:B:137:HIS:HB3	1:B:221:LEU:HD12	1.79	0.62
1:C:59:MET:HA	3:C:502:FMN:C5A	2.30	0.62
1:B:62:TYR:HB2	1:B:148:TRP:CH2	2.35	0.62
1:E:269:LEU:HD11	1:E:288:ALA:HB1	1.82	0.62
1:B:66:ASP:HB3	1:B:68:HIS:HD2	1.65	0.62
1:E:59:MET:HA	3:E:502:FMN:C5A	2.30	0.61
1:B:332:LYS:HB2	1:B:341:VAL:HG21	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:MET:HA	3:B:502:FMN:C5A	2.31	0.61
1:E:4:ILE:HG21	1:G:149:MET:HG2	1.83	0.60
1:G:168:LYS:HE2	1:G:183:ARG:HD2	1.82	0.60
1:B:372:GLN:O	1:C:83:ARG:NH1	2.34	0.60
1:C:59:MET:HA	3:C:502:FMN:N5	2.16	0.60
1:G:332:LYS:HD2	1:G:335:VAL:HG12	1.83	0.60
1:C:93:THR:HG23	1:C:106:VAL:HG12	1.83	0.60
1:G:213:GLU:HB2	1:G:266:PHE:HB2	1.83	0.60
1:B:326:PRO:HA	1:B:329:ILE:HD12	1.84	0.60
1:E:310:GLY:H	1:E:315:GLN:NE2	1.97	0.60
1:G:225:PHE:HA	1:G:231:ASN:HD22	1.66	0.60
1:G:356:LEU:O	1:G:362:LEU:HB2	2.02	0.60
1:B:397:TRP:NE1	3:C:502:FMN:HM72	2.17	0.59
1:G:216:ASN:HD21	1:G:248:PRO:HB3	1.67	0.59
1:E:275:LEU:HD21	1:E:312:HIS:HB3	1.84	0.59
1:B:198:VAL:HG12	1:B:202:LYS:HE3	1.85	0.59
1:C:145:THR:HG21	1:C:151:ASN:O	2.02	0.59
1:B:229:TYR:CE2	1:B:312:HIS:HB2	2.37	0.58
1:G:332:LYS:NZ	1:G:339:MET:O	2.36	0.58
1:G:134:GLN:OE1	1:G:215:HIS:HD2	1.86	0.58
1:G:245:MET:HB3	1:G:249:LEU:HD13	1.86	0.58
1:C:221:LEU:O	1:C:222:LEU:HB2	2.03	0.58
1:B:325:ALA:N	1:B:326:PRO:HD2	2.19	0.58
1:E:236:GLU:HB2	1:E:246:ARG:NH2	2.19	0.58
1:C:19:GLN:HE21	1:C:393:GLY:H	1.51	0.57
1:G:43:ILE:HG23	1:G:53:ARG:CZ	2.34	0.57
1:B:216:ASN:OD1	1:B:222:LEU:HB3	2.05	0.57
1:B:268:ARG:HA	1:B:305:ASP:HB3	1.87	0.56
1:E:133:ILE:HD12	1:E:209:ALA:HB2	1.85	0.56
1:B:60:CYS:N	3:B:502:FMN:H6	2.20	0.56
1:B:80:ILE:HG12	1:B:375:PRO:HB3	1.85	0.56
1:E:237:TYR:HA	1:E:243:ASN:O	2.04	0.56
1:C:139:GLY:HA3	1:C:220:TYR:O	2.06	0.56
1:B:216:ASN:HD21	1:B:248:PRO:HB3	1.70	0.56
1:E:38:LYS:O	1:E:53:ARG:HD2	2.06	0.56
1:E:239:GLY:H	1:E:243:ASN:HB3	1.71	0.56
1:G:390:ALA:HA	1:G:408:PRO:O	2.05	0.56
1:G:341:VAL:HG23	1:G:362:LEU:HD23	1.88	0.56
1:E:329:ILE:HG12	1:E:360:GLU:HB3	1.88	0.56
1:G:245:MET:HE2	1:G:249:LEU:HD11	1.88	0.56
1:B:225:PHE:O	1:B:244:ARG:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:GLU:O	1:B:246:ARG:HD2	2.06	0.55
1:C:198:VAL:HG13	1:C:258:THR:HG21	1.88	0.55
1:G:38:LYS:O	1:G:53:ARG:HD2	2.06	0.55
1:G:100:ARG:HB3	1:G:102:SER:O	2.05	0.55
1:G:215:HIS:CE1	1:G:220:TYR:HD2	2.24	0.55
1:B:4:ILE:HG22	1:B:5:LYS:N	2.21	0.55
1:B:59:MET:HA	3:B:502:FMN:N5	2.22	0.55
1:B:243:ASN:O	1:B:246:ARG:HG2	2.06	0.55
1:E:373:LYS:HD2	1:G:379:TRP:CZ2	2.42	0.55
1:B:156:ALA:HB1	1:B:160:VAL:HG21	1.88	0.55
1:C:146:VAL:CG1	1:C:149:MET:HG3	2.35	0.55
1:E:176:SER:HG	1:E:179:PHE:HD1	1.55	0.55
1:G:69:MET:O	1:G:116:PRO:HB3	2.07	0.55
1:C:100:ARG:HG2	1:C:105:ASP:HB2	1.88	0.55
1:C:303:LEU:HA	1:C:340:LEU:O	2.07	0.55
1:E:367:VAL:HG11	1:E:377:LEU:HD12	1.88	0.55
1:C:390:ALA:HA	1:C:408:PRO:O	2.07	0.55
1:G:38:LYS:HG2	1:G:357:LEU:HB3	1.88	0.55
1:B:260:GLY:HA3	4:E:501:MPD:C1	2.26	0.54
1:E:59:MET:HA	3:E:502:FMN:N5	2.21	0.54
1:E:62:TYR:HB2	1:E:148:TRP:CH2	2.42	0.54
1:C:173:ILE:O	1:C:182:PRO:HG3	2.08	0.54
1:G:193:PHE:CE2	1:G:251:ILE:HD11	2.43	0.54
1:G:245:MET:CE	1:G:249:LEU:HD11	2.38	0.54
1:E:158:GLU:CD	1:E:158:GLU:H	2.11	0.54
1:E:259:VAL:HG13	1:E:263:VAL:HB	1.89	0.54
1:B:110:LYS:HG2	1:B:113:GLN:CD	2.28	0.54
1:B:150:LEU:HD12	1:C:4:ILE:HD13	1.90	0.54
1:G:343:THR:HG21	1:G:356:LEU:HD23	1.90	0.54
1:C:145:THR:HG22	1:C:154:SER:H	1.73	0.53
1:B:137:HIS:O	1:B:220:TYR:HB3	2.08	0.53
1:G:171:SER:HA	1:G:184:ALA:HB2	1.91	0.53
1:B:247:LEU:HB3	1:B:248:PRO:HD3	1.90	0.53
1:B:269:LEU:HD23	1:B:306:VAL:HA	1.91	0.53
1:C:216:ASN:HD21	1:C:248:PRO:HB3	1.72	0.53
1:E:379:TRP:O	1:E:383:GLN:HG3	2.09	0.53
1:E:385:LEU:HB2	1:E:387:VAL:HG23	1.91	0.52
1:C:27:ALA:O	1:C:30:GLN:HG2	2.09	0.52
1:C:274:TRP:CE2	1:C:317:VAL:HG13	2.45	0.52
1:E:62:TYR:HB2	1:E:148:TRP:CZ3	2.45	0.52
1:G:62:TYR:HB2	1:G:148:TRP:CH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ALA:HB3	1:B:12:ILE:CD1	2.36	0.52
1:C:115:ALA:HB3	1:C:116:PRO:HD3	1.91	0.52
1:B:199:ALA:O	1:B:203:ARG:HG2	2.10	0.52
1:B:344:VAL:HG23	1:B:366:LEU:O	2.10	0.52
1:G:59:MET:HA	3:G:501:FMN:C5A	2.40	0.52
1:B:85:PRO:HG2	1:B:88:ILE:CG1	2.38	0.52
1:B:246:ARG:HG3	1:B:247:LEU:H	1.73	0.52
1:C:274:TRP:CG	1:C:317:VAL:HG22	2.44	0.52
1:E:84:GLY:N	1:E:85:PRO:HD3	2.24	0.52
1:E:275:LEU:HD12	1:E:282:THR:HG22	1.91	0.52
1:B:324:GLN:HG3	1:B:344:VAL:O	2.10	0.52
1:E:335:VAL:HG11	1:E:339:MET:HB2	1.92	0.52
1:E:399:PHE:CZ	1:G:369:ARG:HB3	2.45	0.52
1:B:156:ALA:HB1	1:B:160:VAL:CG2	2.40	0.51
1:C:254:LEU:O	1:C:258:THR:HG23	2.10	0.51
1:G:12:ILE:CD1	1:G:16:THR:HG22	2.40	0.51
1:C:43:ILE:HG23	1:C:53:ARG:CZ	2.40	0.51
1:B:170:PRO:HB2	1:B:231:ASN:HD22	1.75	0.51
1:C:228:PRO:HG2	1:C:281:GLU:HB3	1.93	0.51
1:G:114:ILE:CD1	1:G:203:ARG:HB2	2.40	0.51
1:G:137:HIS:O	1:G:220:TYR:HB3	2.10	0.51
1:B:60:CYS:H	3:B:502:FMN:H6	1.75	0.51
1:B:250:LYS:HE3	1:B:254:LEU:HG	1.92	0.51
1:C:167:VAL:HG21	1:C:180:PRO:HG3	1.91	0.51
1:C:347:ILE:HD13	1:C:365:VAL:HG13	1.91	0.51
1:E:310:GLY:N	1:E:315:GLN:HE22	1.99	0.51
1:G:245:MET:HB3	1:G:249:LEU:CD1	2.40	0.51
1:B:4:ILE:HG22	1:B:5:LYS:H	1.76	0.51
1:B:270:SER:HB2	1:B:311:LEU:HD21	1.91	0.51
1:E:137:HIS:O	1:E:220:TYR:HB3	2.11	0.51
1:G:30:GLN:HE22	1:G:388:GLU:H	1.58	0.51
1:B:383:GLN:HB3	1:B:416:LYS:HE3	1.92	0.50
1:C:43:ILE:HG12	1:C:53:ARG:CG	2.41	0.50
1:C:221:LEU:O	1:C:223:ALA:N	2.39	0.50
1:B:296:ALA:HB2	1:B:339:MET:HE2	1.94	0.50
1:E:246:ARG:HH21	1:E:246:ARG:HG3	1.76	0.50
1:G:324:GLN:HG3	1:G:344:VAL:O	2.12	0.50
1:C:145:THR:CG2	1:C:154:SER:H	2.25	0.50
1:E:43:ILE:CD1	1:E:53:ARG:HG2	2.42	0.50
1:E:174:PRO:HG3	1:E:181:ARG:HE	1.76	0.50
1:G:101:ILE:N	1:G:105:ASP:OD2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LEU:HD23	1:B:378:VAL:HG22	1.94	0.50
1:B:216:ASN:CG	1:B:222:LEU:HB3	2.32	0.50
1:B:275:LEU:O	1:B:276:GLY:C	2.50	0.50
1:C:95:VAL:HG11	1:C:197:TRP:CE3	2.47	0.50
1:E:266:PHE:CG	1:E:303:LEU:HD22	2.46	0.50
1:E:392:PRO:O	1:E:396:ARG:HG2	2.12	0.50
1:B:367:VAL:HB	1:B:371:PHE:CE2	2.47	0.49
1:G:108:LEU:O	1:G:203:ARG:HD2	2.12	0.49
1:E:285:LEU:O	1:E:289:VAL:HG23	2.12	0.49
1:G:185:MET:SD	1:G:221:LEU:HD11	2.52	0.49
1:G:286:GLN:HA	1:G:289:VAL:HG22	1.93	0.49
1:C:109:TRP:CD1	1:C:110:LYS:HG2	2.47	0.49
1:G:155:ILE:HD11	1:G:180:PRO:HB3	1.95	0.49
1:G:241:PHE:CE1	1:G:290:ARG:HD3	2.48	0.49
1:E:233:ARG:HB2	1:E:238:GLY:HA3	1.94	0.49
1:E:401:LYS:HE2	1:E:401:LYS:H	1.76	0.49
1:G:215:HIS:CE1	1:G:220:TYR:CD2	3.00	0.49
1:G:225:PHE:HA	1:G:231:ASN:ND2	2.28	0.49
1:E:140:ARG:NH1	1:E:173:ILE:O	2.42	0.49
1:B:97:PRO:HG3	1:B:109:TRP:CE2	2.47	0.48
1:C:341:VAL:CG2	1:C:362:LEU:HD22	2.43	0.48
1:E:51:GLN:NE2	1:E:129:GLN:NE2	2.61	0.48
1:E:252:ALA:HB3	1:E:298:GLN:HE22	1.79	0.48
1:E:151:ASN:HD21	1:G:3:ASP:HB3	1.78	0.48
1:E:373:LYS:HD2	1:G:379:TRP:CE2	2.49	0.48
1:G:291:PHE:O	1:G:295:LEU:HG	2.13	0.48
1:B:158:GLU:CD	1:B:158:GLU:H	2.15	0.48
1:G:274:TRP:CD2	1:G:317:VAL:HA	2.48	0.48
1:B:385:LEU:HB2	1:B:387:VAL:HG23	1.96	0.48
1:C:296:ALA:HB2	1:C:339:MET:HE2	1.95	0.48
1:E:281:GLU:H	1:E:281:GLU:HG2	1.37	0.48
1:G:125:HIS:HE1	1:G:210:ASP:OD2	1.96	0.48
1:C:51:GLN:HE22	1:C:129:GLN:NE2	2.09	0.48
1:B:341:VAL:CG2	1:B:362:LEU:HD22	2.44	0.48
1:C:221:LEU:C	1:C:223:ALA:N	2.67	0.48
1:G:69:MET:CE	1:G:117:ILE:HA	2.43	0.48
1:E:3:ASP:HB2	1:G:151:ASN:ND2	2.29	0.48
1:E:357:LEU:HD21	1:E:365:VAL:HG23	1.94	0.48
1:G:106:VAL:HG12	5:G:607:HOH:O	2.13	0.48
3:G:501:FMN:H2'	3:G:501:FMN:C9	2.43	0.48
1:C:342:ALA:HB2	1:C:364:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:34:LYS:HE3	1:G:34:LYS:HB2	1.56	0.48
1:G:349:ASP:OD2	1:G:351:LYS:HB2	2.14	0.48
1:E:181:ARG:HD3	1:E:182:PRO:HD2	1.96	0.47
1:G:399:PHE:HB3	1:G:414:VAL:HG11	1.96	0.47
1:B:48:LEU:HD23	1:B:50:PHE:CZ	2.48	0.47
1:B:233:ARG:HD3	1:B:237:TYR:HB2	1.95	0.47
1:E:40:PHE:CE1	1:E:389:VAL:HG11	2.49	0.47
1:B:59:MET:N	5:B:602:HOH:O	2.46	0.47
1:C:216:ASN:ND2	1:C:248:PRO:HB3	2.29	0.47
1:E:185:MET:HE2	1:E:185:MET:HB3	1.71	0.47
1:B:190:ILE:O	1:B:194:LYS:HG3	2.15	0.47
1:E:21:THR:CG2	1:E:408:PRO:HG3	2.36	0.47
1:B:232:LYS:HB2	1:B:232:LYS:HE3	1.52	0.47
1:C:149:MET:O	1:C:152:HIS:HB3	2.15	0.47
1:C:221:LEU:C	1:C:223:ALA:H	2.17	0.47
1:E:190:ILE:O	1:E:194:LYS:HG3	2.14	0.47
1:E:298:GLN:HE21	1:E:300:ALA:HB3	1.79	0.47
1:B:38:LYS:O	1:B:41:GLN:HB2	2.15	0.47
3:C:502:FMN:H5'2	3:C:502:FMN:H2'	1.57	0.47
1:E:368:GLY:HA3	3:E:502:FMN:H5'1	1.97	0.47
1:E:377:LEU:HD23	1:E:377:LEU:HA	1.72	0.47
1:G:12:ILE:HD11	1:G:16:THR:HG22	1.95	0.47
1:G:138:ALA:HB3	1:G:142:ALA:HB2	1.96	0.47
1:B:202:LYS:O	1:B:206:VAL:HG23	2.13	0.47
1:E:96:GLN:HE21	1:E:137:HIS:CD2	2.33	0.47
1:C:158:GLU:HG3	1:C:164:PRO:HD2	1.96	0.46
1:E:397:TRP:CZ2	3:G:501:FMN:HM72	2.50	0.46
1:G:58:PRO:HD3	1:G:89:MET:SD	2.55	0.46
1:B:12:ILE:HD12	1:B:14:TYR:O	2.16	0.46
1:E:114:ILE:HG23	1:E:207:ALA:HB2	1.96	0.46
1:G:205:LEU:HD11	1:G:259:VAL:HG12	1.98	0.46
1:E:227:THR:HB	1:E:229:TYR:CZ	2.49	0.46
1:E:60:CYS:N	3:E:502:FMN:H6	2.31	0.46
1:E:397:TRP:CE2	3:G:501:FMN:HM72	2.50	0.46
1:E:247:LEU:HB3	1:E:248:PRO:HD3	1.97	0.46
1:B:397:TRP:CE2	3:C:502:FMN:HM72	2.51	0.46
1:E:298:GLN:HG2	1:E:300:ALA:H	1.80	0.46
1:B:90:ILE:HD12	1:B:133:ILE:HG12	1.97	0.46
1:C:54:LEU:HD23	1:C:378:VAL:HG22	1.97	0.46
1:G:197:TRP:NE1	1:G:255:THR:OG1	2.44	0.46
1:G:266:PHE:CD1	1:G:303:LEU:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:TRP:HE1	3:C:502:FMN:HM72	1.78	0.46
1:C:110:LYS:HD3	1:C:112:SER:OG	2.15	0.46
1:E:250:LYS:HD2	1:E:254:LEU:HG	1.98	0.46
1:E:275:LEU:O	1:E:276:GLY:C	2.54	0.46
1:C:216:ASN:ND2	1:C:222:LEU:HB3	2.31	0.45
1:C:392:PRO:O	1:C:396:ARG:HG2	2.16	0.45
1:E:51:GLN:NE2	1:E:86:GLY:HA2	2.31	0.45
1:B:177:GLU:HG2	1:B:178:THR:N	2.31	0.45
1:B:186:THR:O	1:B:189:ASP:HB2	2.16	0.45
1:B:341:VAL:HG21	1:B:362:LEU:HD22	1.99	0.45
1:C:156:ALA:O	1:C:162:GLY:HA3	2.16	0.45
1:C:202:LYS:O	1:C:206:VAL:HG23	2.17	0.45
1:C:387:VAL:O	1:C:412:PRO:HG3	2.15	0.45
1:E:401:LYS:HE2	1:E:401:LYS:N	2.31	0.45
1:G:27:ALA:O	1:G:30:GLN:HG2	2.16	0.45
1:G:51:GLN:HE22	1:G:129:GLN:HE22	1.64	0.45
1:G:240:SER:H	1:G:243:ASN:HB2	1.82	0.45
1:G:168:LYS:HA	1:G:168:LYS:HD2	1.64	0.45
1:B:50:PHE:CD2	1:B:87:LEU:HB3	2.52	0.45
1:C:173:ILE:HD11	1:C:232:LYS:HD3	1.99	0.45
1:E:148:TRP:CZ3	1:G:394:GLN:HG3	2.51	0.45
1:E:216:ASN:ND2	1:E:222:LEU:HB3	2.32	0.45
1:B:201:ALA:O	1:B:205:LEU:HG	2.16	0.45
1:C:69:MET:HG2	1:C:73:HIS:CG	2.52	0.45
1:C:85:PRO:HA	1:C:378:VAL:HG21	1.98	0.45
1:E:166:ASN:HA	1:E:183:ARG:NH2	2.25	0.45
1:B:198:VAL:O	1:B:202:LYS:HG3	2.17	0.45
1:E:109:TRP:NE1	1:E:110:LYS:HD3	2.32	0.45
1:G:227:THR:CG2	1:G:311:LEU:HD22	2.46	0.45
1:G:274:TRP:CE3	1:G:317:VAL:HA	2.52	0.45
1:B:193:PHE:CZ	1:B:221:LEU:HD21	2.51	0.45
1:C:357:LEU:HD21	1:C:365:VAL:HG23	1.99	0.45
1:G:32:SER:C	1:G:34:LYS:H	2.20	0.45
1:G:332:LYS:HB2	1:G:341:VAL:HG21	1.98	0.45
1:B:28:ASN:HB3	1:B:29:PRO:HD3	1.99	0.45
1:G:307:SER:OG	1:G:308:SER:N	2.50	0.45
1:B:357:LEU:HD21	1:B:365:VAL:HG23	1.99	0.45
1:E:155:ILE:HG12	1:E:180:PRO:HD3	1.98	0.45
1:E:415:TYR:CE2	1:G:348:ARG:HG2	2.52	0.45
1:G:97:PRO:HG3	1:G:109:TRP:CE2	2.52	0.45
1:B:43:ILE:HG23	1:B:53:ARG:NH2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ARG:HH21	1:C:119:ARG:HH11	1.64	0.44
1:E:259:VAL:HG22	1:E:263:VAL:HG11	1.99	0.44
1:B:241:PHE:HA	1:B:244:ARG:NH1	2.32	0.44
1:G:5:LYS:HE3	1:G:5:LYS:HB3	1.42	0.44
1:E:188:ASP:O	1:E:192:GLU:HG3	2.17	0.44
1:G:146:VAL:HG22	1:G:149:MET:HB2	1.98	0.44
1:G:227:THR:HG21	1:G:311:LEU:HD22	2.00	0.44
1:G:241:PHE:CZ	1:G:290:ARG:HD3	2.51	0.44
1:B:137:HIS:O	1:B:221:LEU:HD12	2.18	0.44
1:C:57:SER:OG	1:C:58:PRO:HD2	2.17	0.44
1:E:51:GLN:NE2	1:E:129:GLN:HE21	2.15	0.44
1:E:260:GLY:HA3	4:E:501:MPD:O2	2.17	0.44
1:E:303:LEU:HA	1:E:340:LEU:O	2.18	0.44
3:B:502:FMN:HM72	1:C:397:TRP:CZ2	2.52	0.44
1:C:367:VAL:HG11	1:C:377:LEU:HD12	2.00	0.44
1:B:389:VAL:O	1:B:409:PHE:HA	2.18	0.44
1:G:28:ASN:HB3	1:G:29:PRO:HD3	2.00	0.44
1:G:254:LEU:O	1:G:258:THR:HG22	2.18	0.44
1:G:415:TYR:HB3	1:G:416:LYS:H	1.68	0.44
1:B:108:LEU:HD12	1:B:108:LEU:HA	1.73	0.44
1:B:170:PRO:HG3	1:B:224:SER:HB3	1.99	0.44
1:C:274:TRP:CD1	1:C:317:VAL:HG22	2.53	0.44
1:G:69:MET:HE3	1:G:117:ILE:HA	1.99	0.44
1:B:74:LEU:HD23	1:C:74:LEU:HD23	1.99	0.44
1:C:176:SER:H	1:C:179:PHE:HB2	1.83	0.44
1:C:275:LEU:HD11	1:C:312:HIS:ND1	2.32	0.44
1:E:150:LEU:H	1:E:150:LEU:HG	1.41	0.44
1:G:185:MET:HB3	1:G:189:ASP:HB2	1.99	0.44
1:G:286:GLN:CD	1:G:286:GLN:H	2.20	0.44
1:C:176:SER:HG	1:C:178:THR:HG23	1.83	0.43
3:C:502:FMN:H2'	3:C:502:FMN:H9	2.00	0.43
1:G:48:LEU:HD23	1:G:48:LEU:HA	1.77	0.43
1:C:10:LYS:HD2	1:C:10:LYS:HA	1.55	0.43
1:E:12:ILE:HG22	1:E:122:GLU:HG2	1.99	0.43
1:B:146:VAL:HG22	1:B:149:MET:HB2	2.00	0.43
1:B:292:ALA:HA	1:B:295:LEU:HD12	2.00	0.43
1:C:401:LYS:HB3	1:C:401:LYS:HE2	1.33	0.43
1:E:275:LEU:HD11	1:E:312:HIS:ND1	2.33	0.43
1:B:284:ASP:OD1	1:B:284:ASP:N	2.52	0.43
1:C:143:SER:HB2	1:C:163:TRP:CE2	2.53	0.43
1:C:172:ASP:HA	1:C:182:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:HIS:HE1	1:B:210:ASP:OD2	2.00	0.43
1:C:385:LEU:HB2	1:C:387:VAL:HG23	2.01	0.43
1:G:192:GLU:H	1:G:192:GLU:HG3	1.37	0.43
1:G:338:ARG:CZ	1:G:338:ARG:HA	2.49	0.43
1:E:114:ILE:HD11	1:E:203:ARG:HG2	2.01	0.43
1:G:232:LYS:HE3	1:G:232:LYS:HB3	1.66	0.43
1:B:23:ALA:HB2	1:B:392:PRO:HD3	2.01	0.43
1:B:222:LEU:HD12	1:B:222:LEU:HA	1.79	0.43
1:E:237:TYR:CD1	1:E:246:ARG:HB3	2.54	0.43
1:G:226:LEU:HD11	1:G:245:MET:HA	2.00	0.43
1:B:43:ILE:CG1	1:B:53:ARG:HG3	2.48	0.43
1:B:150:LEU:H	1:B:150:LEU:HG	1.65	0.43
1:C:79:GLY:O	1:C:83:ARG:HD2	2.18	0.43
1:E:46:ARG:HD3	1:E:261:GLU:O	2.18	0.43
1:E:61:GLN:O	1:G:394:GLN:HG2	2.19	0.43
1:E:160:VAL:HG23	1:G:5:LYS:HA	2.01	0.42
1:E:352:LEU:HD22	1:E:356:LEU:HG	2.01	0.42
3:G:501:FMN:H2'	3:G:501:FMN:H9	2.01	0.42
1:B:233:ARG:C	1:B:235:ASP:H	2.21	0.42
1:E:274:TRP:CD1	1:E:317:VAL:HG12	2.54	0.42
1:E:388:GLU:H	1:E:388:GLU:HG3	1.66	0.42
1:B:43:ILE:HG12	1:B:53:ARG:HG3	2.00	0.42
1:C:274:TRP:CE3	1:C:317:VAL:HA	2.53	0.42
1:E:38:LYS:HA	1:E:41:GLN:CD	2.40	0.42
1:B:40:PHE:CE2	1:B:389:VAL:HG11	2.54	0.42
1:C:100:ARG:HB3	1:C:102:SER:O	2.19	0.42
1:C:348:ARG:HB2	1:C:348:ARG:CZ	2.48	0.42
1:E:390:ALA:HA	1:E:408:PRO:O	2.19	0.42
1:G:224:SER:HA	1:G:227:THR:OG1	2.19	0.42
1:C:166:ASN:OD1	1:C:168:LYS:HE2	2.19	0.42
1:E:38:LYS:HD3	1:E:357:LEU:HB3	2.01	0.42
1:G:155:ILE:CD1	1:G:180:PRO:HB3	2.49	0.42
1:G:241:PHE:CD1	1:G:290:ARG:HD3	2.55	0.42
1:C:69:MET:HA	1:C:73:HIS:CE1	2.55	0.42
1:E:373:LYS:HE3	1:G:415:TYR:HB2	2.01	0.42
1:G:245:MET:HE1	1:G:294:ALA:CB	2.48	0.42
1:B:85:PRO:HG2	1:B:88:ILE:HG13	2.00	0.42
1:C:38:LYS:HD3	1:C:357:LEU:HB3	2.01	0.42
1:E:233:ARG:HB2	1:E:238:GLY:CA	2.49	0.42
1:E:321:PRO:HA	1:E:346:HIS:HB3	2.02	0.42
1:E:344:VAL:HG23	1:E:366:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:172:ASP:C	1:G:182:PRO:HG2	2.40	0.42
1:E:151:ASN:O	1:E:152:HIS:C	2.58	0.42
1:G:44:THR:HA	1:G:49:THR:HA	2.02	0.42
1:B:175:PHE:HB3	1:B:179:PHE:CG	2.54	0.42
1:B:285:LEU:HG	1:B:327:PHE:HD1	1.83	0.42
1:E:415:TYR:HA	1:G:348:ARG:NH2	2.34	0.42
1:G:236:GLU:HB2	1:G:246:ARG:NE	2.35	0.42
1:B:274:TRP:CD2	1:B:317:VAL:HA	2.55	0.41
1:C:215:HIS:CE1	1:C:217:ALA:HB3	2.54	0.41
1:E:173:ILE:O	1:E:182:PRO:HG3	2.20	0.41
1:G:51:GLN:HG2	1:G:52:ASN:ND2	2.34	0.41
1:G:67:GLY:HA2	1:G:105:ASP:O	2.19	0.41
1:G:284:ASP:OD1	1:G:286:GLN:HB2	2.19	0.41
1:B:100:ARG:HD3	1:B:109:TRP:CH2	2.55	0.41
1:B:215:HIS:HE1	1:B:218:HIS:ND1	2.17	0.41
1:C:41:GLN:HA	1:C:42:PRO:HD3	1.92	0.41
1:G:98:GLU:CD	1:G:98:GLU:H	2.23	0.41
1:E:217:ALA:HB2	1:E:269:LEU:HA	2.01	0.41
1:E:392:PRO:HG2	1:E:395:ILE:HD12	2.03	0.41
1:G:198:VAL:O	1:G:202:LYS:HB2	2.21	0.41
1:G:226:LEU:HB3	1:G:283:TRP:CZ3	2.55	0.41
1:G:271:ALA:HB1	1:G:285:LEU:HD13	2.02	0.41
1:B:82:GLN:HG2	1:B:392:PRO:HG3	2.03	0.41
1:E:148:TRP:CH2	1:G:394:GLN:HG3	2.56	0.41
1:E:245:MET:HG2	1:E:291:PHE:CD1	2.55	0.41
1:G:51:GLN:HG2	1:G:52:ASN:HD22	1.85	0.41
1:B:259:VAL:HG21	1:B:265:VAL:CG2	2.51	0.41
1:C:77:LEU:HD23	1:C:77:LEU:HA	1.88	0.41
1:E:262:HIS:HD2	4:E:501:MPD:C1	2.23	0.41
1:E:146:VAL:HG23	1:E:147:PRO:HD2	2.01	0.41
1:G:325:ALA:N	1:G:326:PRO:CD	2.84	0.41
1:G:411:ASP:C	1:G:413:SER:H	2.23	0.41
1:C:69:MET:HG2	1:C:73:HIS:CE1	2.55	0.41
1:E:23:ALA:HB2	1:E:392:PRO:HD3	2.03	0.41
1:E:411:ASP:HB2	1:E:412:PRO:HD2	2.02	0.41
1:G:205:LEU:HD11	1:G:259:VAL:HA	2.03	0.41
1:B:28:ASN:CB	1:B:29:PRO:HD3	2.51	0.41
1:B:200:ALA:O	1:B:203:ARG:HG3	2.21	0.41
1:B:231:ASN:HD21	1:B:233:ARG:CD	2.34	0.41
1:B:237:TYR:HA	1:B:243:ASN:O	2.21	0.41
1:C:51:GLN:NE2	1:C:129:GLN:HE22	2.14	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:CYS:HA	1:C:91:GLU:HB2	2.02	0.41
1:E:130:LYS:HA	1:E:210:ASP:OD2	2.20	0.41
1:G:286:GLN:O	1:G:287:HIS:C	2.58	0.41
1:G:347:ILE:H	1:G:347:ILE:HG12	1.59	0.41
1:E:379:TRP:CE2	1:G:373:LYS:HE2	2.55	0.41
1:E:397:TRP:NE1	3:G:501:FMN:HM72	2.36	0.41
1:B:246:ARG:HG3	1:B:247:LEU:N	2.35	0.41
1:C:146:VAL:HG23	1:C:147:PRO:HD2	2.02	0.41
1:E:27:ALA:O	1:E:30:GLN:HG2	2.21	0.41
1:G:202:LYS:O	1:G:206:VAL:HG23	2.21	0.41
1:C:163:TRP:N	1:C:164:PRO:HD3	2.36	0.40
1:E:369:ARG:O	1:G:399:PHE:HZ	2.03	0.40
1:C:167:VAL:HG21	1:C:180:PRO:CG	2.51	0.40
1:E:233:ARG:C	1:E:238:GLY:HA3	2.41	0.40
1:C:87:LEU:HD13	1:C:211:PHE:CZ	2.56	0.40
1:G:3:ASP:HB3	1:G:4:ILE:H	1.77	0.40
1:B:66:ASP:HB3	1:B:68:HIS:CD2	2.52	0.40
1:C:5:LYS:HG2	1:C:6:VAL:N	2.36	0.40
1:C:107:GLY:HA3	1:C:109:TRP:CZ3	2.56	0.40
1:E:96:GLN:NE2	1:E:137:HIS:CD2	2.89	0.40
1:C:69:MET:O	1:C:116:PRO:HB3	2.21	0.40
1:E:109:TRP:HE1	1:E:110:LYS:HD3	1.87	0.40
1:E:401:LYS:HB2	1:E:404:ARG:NH1	2.35	0.40
1:G:150:LEU:H	1:G:150:LEU:HG	1.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	401/422 (95%)	371 (92%)	30 (8%)	0	<a href="#">100</a> <a href="#">100</a>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	409/422 (97%)	381 (93%)	27 (7%)	1 (0%)	47	78
1	E	403/422 (96%)	370 (92%)	33 (8%)	0	100	100
1	G	399/422 (94%)	354 (89%)	45 (11%)	0	100	100
All	All	1612/1688 (96%)	1476 (92%)	135 (8%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	30	GLN

### 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	B	323/337 (96%)	288 (89%)	35 (11%)	6	19
1	C	329/337 (98%)	300 (91%)	29 (9%)	10	29
1	E	325/337 (96%)	299 (92%)	26 (8%)	12	34
1	G	324/337 (96%)	290 (90%)	34 (10%)	7	20
All	All	1301/1348 (96%)	1177 (90%)	124 (10%)	8	25

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	28	ASN
1	B	43	ILE
1	B	53	ARG
1	B	89	MET
1	B	149	MET
1	B	155	ILE
1	B	157	THR
1	B	159	ASN
1	B	160	VAL
1	B	168	LYS

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Mol	Chain	Res	Type
1	B	203	ARG
1	B	213	GLU
1	B	215	HIS
1	B	221	LEU
1	B	222	LEU
1	B	229	TYR
1	B	232	LYS
1	B	233	ARG
1	B	246	ARG
1	B	250	LYS
1	B	269	LEU
1	B	275	LEU
1	B	284	ASP
1	B	285	LEU
1	B	308	SER
1	B	324	GLN
1	B	339	MET
1	B	356	LEU
1	B	386	ASP
1	B	394	GLN
1	B	396	ARG
1	B	401	LYS
1	B	405	ARG
1	B	407	THR
1	B	416	LYS
1	C	34	LYS
1	C	36	ILE
1	C	43	ILE
1	C	46	ARG
1	C	48	LEU
1	C	83	ARG
1	C	88	ILE
1	C	89	MET
1	C	110	LYS
1	C	159	ASN
1	C	160	VAL
1	C	168	LYS
1	C	172	ASP
1	C	178	THR
1	C	187	GLN
1	C	188	ASP
1	C	191	ARG

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Mol	Chain	Res	Type
1	C	215	HIS
1	C	250	LYS
1	C	277	SER
1	C	278	THR
1	C	339	MET
1	C	340	LEU
1	C	377	LEU
1	C	386	ASP
1	C	401	LYS
1	C	405	ARG
1	C	407	THR
1	C	416	LYS
1	E	21	THR
1	E	43	ILE
1	E	46	ARG
1	E	74	LEU
1	E	83	ARG
1	E	87	LEU
1	E	149	MET
1	E	150	LEU
1	E	159	ASN
1	E	183	ARG
1	E	215	HIS
1	E	229	TYR
1	E	232	LYS
1	E	246	ARG
1	E	247	LEU
1	E	269	LEU
1	E	280	THR
1	E	281	GLU
1	E	282	THR
1	E	315	GLN
1	E	355	ARG
1	E	359	GLU
1	E	377	LEU
1	E	388	GLU
1	E	405	ARG
1	E	407	THR
1	G	3	ASP
1	G	4	ILE
1	G	5	LYS
1	G	28	ASN

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Mol	Chain	Res	Type
1	G	34	LYS
1	G	46	ARG
1	G	48	LEU
1	G	83	ARG
1	G	111	ASP
1	G	130	LYS
1	G	131	ILE
1	G	149	MET
1	G	150	LEU
1	G	168	LYS
1	G	173	ILE
1	G	191	ARG
1	G	192	GLU
1	G	194	LYS
1	G	202	LYS
1	G	226	LEU
1	G	229	TYR
1	G	240	SER
1	G	280	THR
1	G	282	THR
1	G	284	ASP
1	G	290	ARG
1	G	335	VAL
1	G	338	ARG
1	G	339	MET
1	G	347	ILE
1	G	349	ASP
1	G	362	LEU
1	G	401	LYS
1	G	416	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	68	HIS
1	B	125	HIS
1	B	129	GLN
1	B	215	HIS
1	B	216	ASN
1	B	231	ASN
1	B	262	HIS
1	B	312	HIS

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Mol	Chain	Res	Type
1	B	324	GLN
1	C	19	GLN
1	C	129	GLN
1	C	159	ASN
1	C	187	GLN
1	C	216	ASN
1	C	312	HIS
1	C	315	GLN
1	C	346	HIS
1	E	30	GLN
1	E	51	GLN
1	E	96	GLN
1	E	129	GLN
1	E	151	ASN
1	E	216	ASN
1	E	231	ASN
1	E	262	HIS
1	E	298	GLN
1	E	315	GLN
1	E	346	HIS
1	G	28	ASN
1	G	30	GLN
1	G	82	GLN
1	G	104	GLN
1	G	129	GLN
1	G	152	HIS
1	G	215	HIS
1	G	216	ASN
1	G	231	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MPD	E	501	-	7,7,7	0.36	0	9,10,10	1.41	1 (11%)
3	FMN	B	502	-	31,33,33	1.36	4 (12%)	40,50,50	1.77	7 (17%)
2	SO4	B	501	-	4,4,4	0.17	0	6,6,6	0.27	0
3	FMN	C	502	-	31,33,33	1.63	5 (16%)	40,50,50	2.51	17 (42%)
3	FMN	E	502	-	31,33,33	1.42	5 (16%)	40,50,50	2.15	14 (35%)
2	SO4	G	502	-	4,4,4	0.12	0	6,6,6	0.13	0
2	SO4	E	503	-	4,4,4	0.23	0	6,6,6	0.25	0
2	SO4	C	501	-	4,4,4	0.19	0	6,6,6	0.46	0
3	FMN	G	501	-	31,33,33	1.52	5 (16%)	40,50,50	1.91	10 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	E	501	-	-	1/5/5/5	-
3	FMN	B	502	-	-	10/18/18/18	0/3/3/3
3	FMN	C	502	-	-	12/18/18/18	0/3/3/3
3	FMN	E	502	-	-	12/18/18/18	0/3/3/3
3	FMN	G	501	-	-	3/18/18/18	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	501	FMN	C10-N1	4.44	1.39	1.33
3	C	502	FMN	C1'-N10	4.28	1.52	1.48
3	C	502	FMN	C4-N3	3.98	1.40	1.33
3	B	502	FMN	C10-N1	3.86	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	FMN	C4A-N5	3.59	1.38	1.33
3	E	502	FMN	C10-N1	3.44	1.37	1.33
3	G	501	FMN	C4A-N5	3.41	1.38	1.33
3	B	502	FMN	C4A-N5	3.31	1.38	1.33
3	G	501	FMN	C1'-N10	3.17	1.51	1.48
3	E	502	FMN	C4-N3	3.14	1.38	1.33
3	B	502	FMN	C4-N3	3.12	1.38	1.33
3	C	502	FMN	C5A-N5	3.01	1.40	1.35
3	G	501	FMN	C4-N3	3.00	1.38	1.33
3	E	502	FMN	C4A-N5	2.80	1.37	1.33
3	C	502	FMN	C10-N1	2.78	1.36	1.33
3	E	502	FMN	C2'-C3'	-2.64	1.48	1.53
3	G	501	FMN	C5A-N5	2.27	1.39	1.35
3	B	502	FMN	C4A-C4	-2.19	1.37	1.41
3	E	502	FMN	C5A-N5	2.13	1.38	1.35

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	FMN	C1'-N10-C9A	6.50	123.41	118.29
3	B	502	FMN	C2-N3-C4	6.32	120.47	115.14
3	G	501	FMN	C2-N3-C4	5.59	119.86	115.14
3	E	502	FMN	C2-N3-C4	5.48	119.77	115.14
3	C	502	FMN	C5A-C9A-N10	5.17	121.46	117.72
3	C	502	FMN	P-O5'-C5'	5.14	132.46	118.30
3	C	502	FMN	C2-N3-C4	5.09	119.44	115.14
3	G	501	FMN	C4'-C3'-C2'	-4.65	103.68	113.36
3	E	502	FMN	C1'-N10-C9A	4.57	121.89	118.29
3	C	502	FMN	O4'-C4'-C5'	-4.52	99.76	109.92
3	B	502	FMN	C1'-N10-C9A	4.34	121.71	118.29
3	E	502	FMN	O4'-C4'-C5'	-4.09	100.73	109.92
3	C	502	FMN	C1'-C2'-C3'	3.96	120.85	109.79
3	E	502	FMN	C4A-N5-C5A	3.93	120.70	116.77
3	E	502	FMN	O3'-C3'-C2'	-3.60	100.11	108.81
3	G	501	FMN	C4A-N5-C5A	3.54	120.31	116.77
3	G	501	FMN	O4'-C4'-C3'	-3.47	100.67	109.10
3	C	502	FMN	O2'-C2'-C3'	-3.40	100.82	109.10
3	G	501	FMN	O3P-P-O5'	3.38	115.72	106.73
3	B	502	FMN	C4A-N5-C5A	3.21	119.98	116.77
3	G	501	FMN	C1'-C2'-C3'	3.11	118.48	109.79
4	E	501	MPD	O2-C2-C1	-2.96	98.58	108.08
3	E	502	FMN	P-O5'-C5'	-2.95	110.18	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	FMN	O5'-P-O1P	2.89	114.58	106.47
3	E	502	FMN	C10-C4A-N5	-2.81	119.31	121.26
3	E	502	FMN	O5'-C5'-C4'	-2.79	101.92	109.36
3	G	501	FMN	O2'-C2'-C1'	2.77	116.26	109.59
3	C	502	FMN	C4'-C3'-C2'	-2.71	107.72	113.36
3	B	502	FMN	C4A-C4-N3	-2.70	119.75	123.43
3	C	502	FMN	O3'-C3'-C2'	2.67	115.26	108.81
3	C	502	FMN	O3P-P-O5'	2.66	113.82	106.73
3	G	501	FMN	C1'-N10-C9A	2.65	120.38	118.29
3	C	502	FMN	C9A-C5A-N5	-2.64	118.23	122.36
3	E	502	FMN	C4A-C4-N3	-2.61	119.86	123.43
3	B	502	FMN	O5'-C5'-C4'	-2.60	102.43	109.36
3	E	502	FMN	C4'-C3'-C2'	-2.54	108.07	113.36
3	C	502	FMN	C9A-N10-C10	-2.54	118.59	121.91
3	E	502	FMN	O3'-C3'-C4'	2.53	114.92	108.81
3	G	501	FMN	C10-C4A-N5	-2.48	119.54	121.26
3	E	502	FMN	O4'-C4'-C3'	2.44	115.04	109.10
3	B	502	FMN	O4'-C4'-C5'	-2.42	104.48	109.92
3	B	502	FMN	C5A-C9A-N10	2.37	119.44	117.72
3	C	502	FMN	C4A-N5-C5A	2.29	119.06	116.77
3	C	502	FMN	C6-C5A-N5	2.28	121.56	119.05
3	C	502	FMN	O4'-C4'-C3'	2.27	114.61	109.10
3	G	501	FMN	C4A-C4-N3	-2.21	120.41	123.43
3	E	502	FMN	O5'-P-O1P	-2.19	100.32	106.47
3	C	502	FMN	C4A-C4-N3	-2.11	120.55	123.43
3	E	502	FMN	O2P-P-O5'	2.09	112.31	106.73

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	FMN	C1'-C2'-C3'-O3'
3	B	502	FMN	C1'-C2'-C3'-C4'
3	B	502	FMN	O2'-C2'-C3'-O3'
3	B	502	FMN	O2'-C2'-C3'-C4'
3	B	502	FMN	C5'-O5'-P-O1P
3	B	502	FMN	C5'-O5'-P-O2P
3	B	502	FMN	C5'-O5'-P-O3P
3	C	502	FMN	C1'-C2'-C3'-O3'
3	C	502	FMN	C1'-C2'-C3'-C4'
3	C	502	FMN	O2'-C2'-C3'-O3'
3	C	502	FMN	O2'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
3	C	502	FMN	C2'-C3'-C4'-O4'
3	C	502	FMN	C2'-C3'-C4'-C5'
3	C	502	FMN	O3'-C3'-C4'-O4'
3	C	502	FMN	C4'-C5'-O5'-P
3	C	502	FMN	C5'-O5'-P-O2P
3	C	502	FMN	C5'-O5'-P-O3P
3	E	502	FMN	N10-C1'-C2'-O2'
3	E	502	FMN	C1'-C2'-C3'-O3'
3	E	502	FMN	C1'-C2'-C3'-C4'
3	E	502	FMN	O2'-C2'-C3'-O3'
3	E	502	FMN	O2'-C2'-C3'-C4'
3	E	502	FMN	C3'-C4'-C5'-O5'
3	E	502	FMN	O4'-C4'-C5'-O5'
3	E	502	FMN	C5'-O5'-P-O2P
3	E	502	FMN	C5'-O5'-P-O3P
3	C	502	FMN	O3'-C3'-C4'-C5'
3	G	501	FMN	O2'-C2'-C3'-O3'
3	G	501	FMN	O2'-C2'-C3'-C4'
3	B	502	FMN	O4'-C4'-C5'-O5'
3	B	502	FMN	C3'-C4'-C5'-O5'
3	E	502	FMN	C5'-O5'-P-O1P
3	G	501	FMN	C4'-C5'-O5'-P
3	E	502	FMN	N10-C1'-C2'-C3'
3	E	502	FMN	C2'-C3'-C4'-O4'
3	B	502	FMN	O3'-C3'-C4'-O4'
3	C	502	FMN	C5'-O5'-P-O1P
4	E	501	MPD	C2-C3-C4-C5

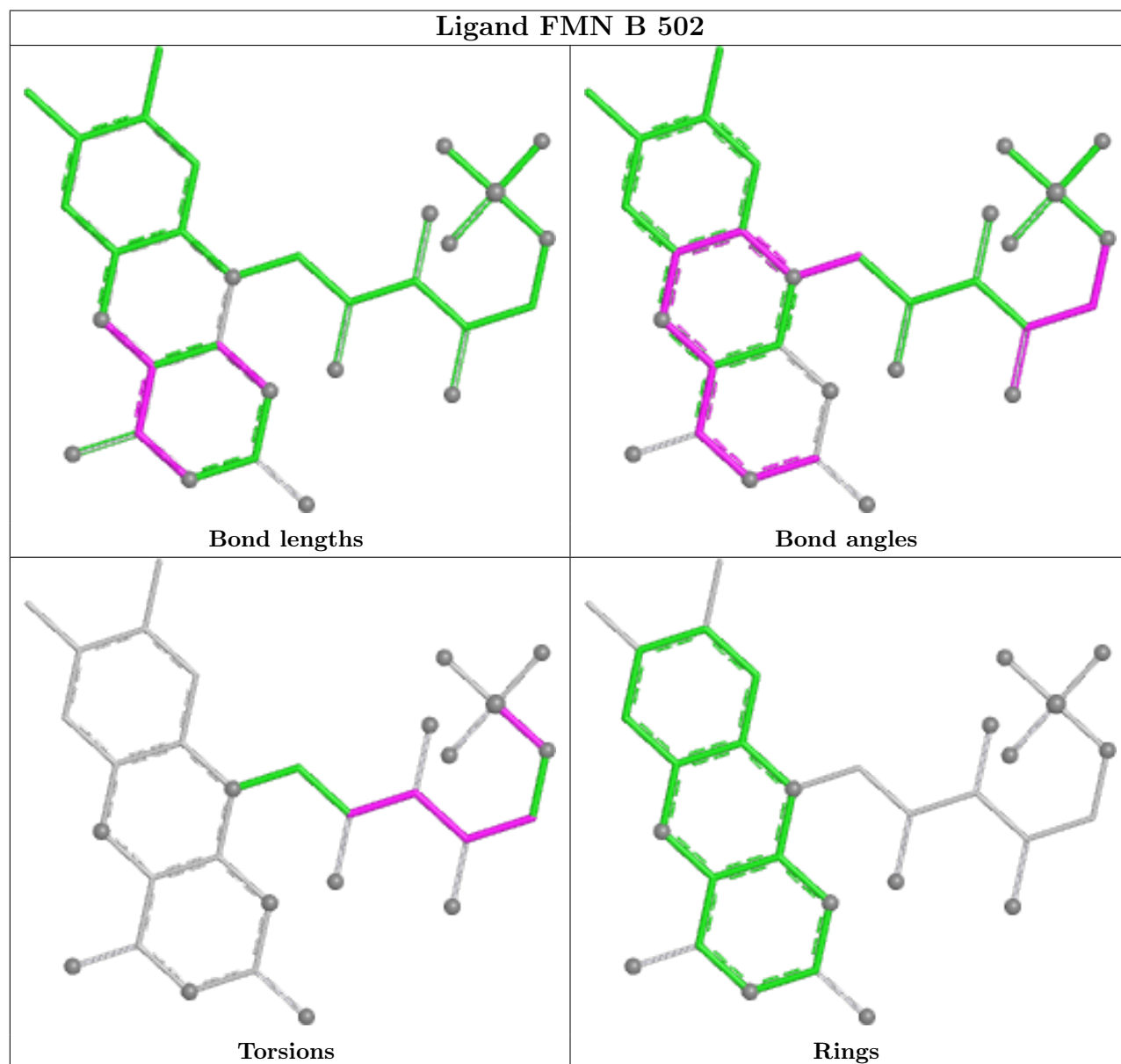
There are no ring outliers.

5 monomers are involved in 29 short contacts:

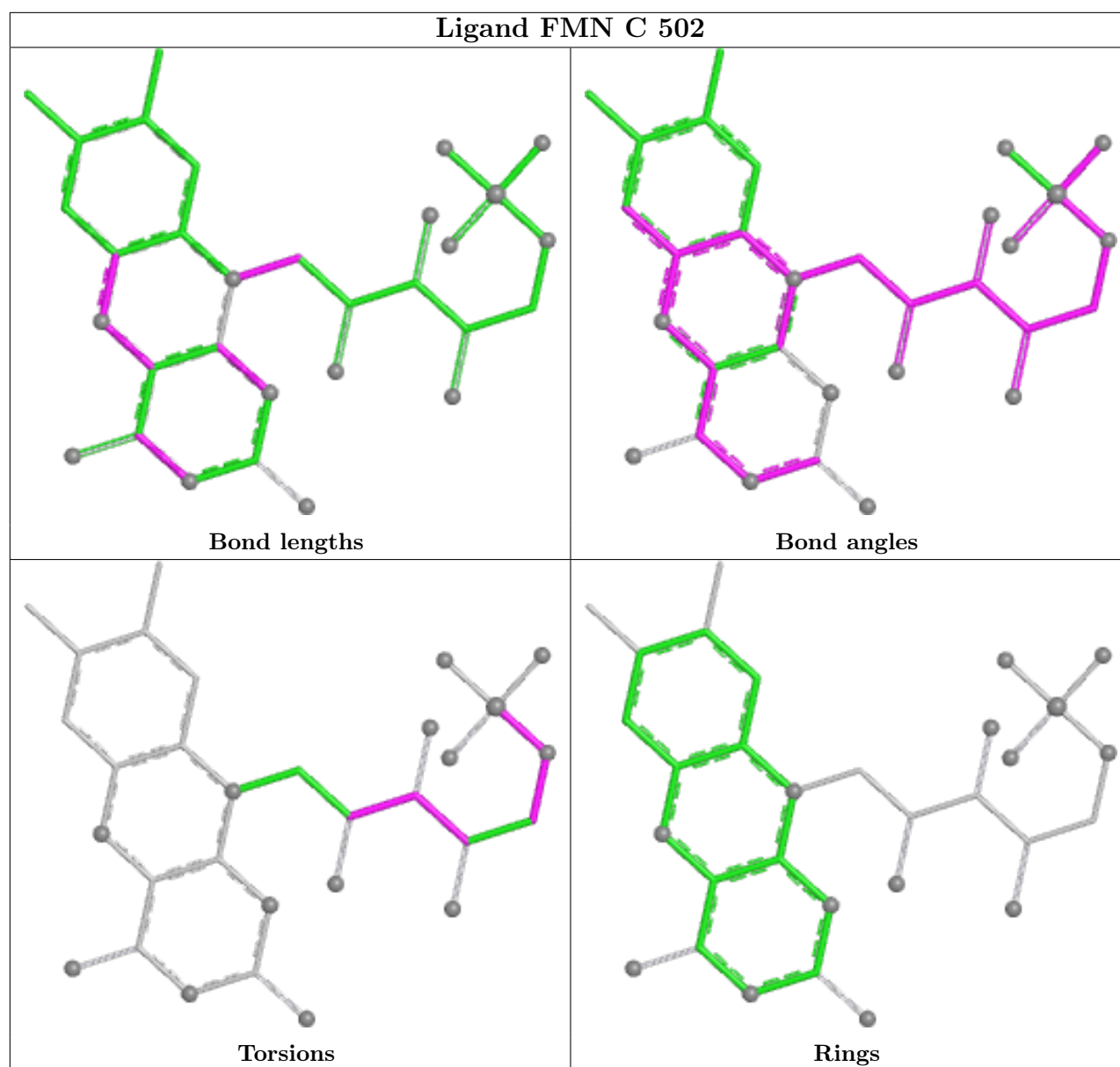
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	501	MPD	6	0
3	B	502	FMN	5	0
3	C	502	FMN	7	0
3	E	502	FMN	4	0
3	G	501	FMN	7	0

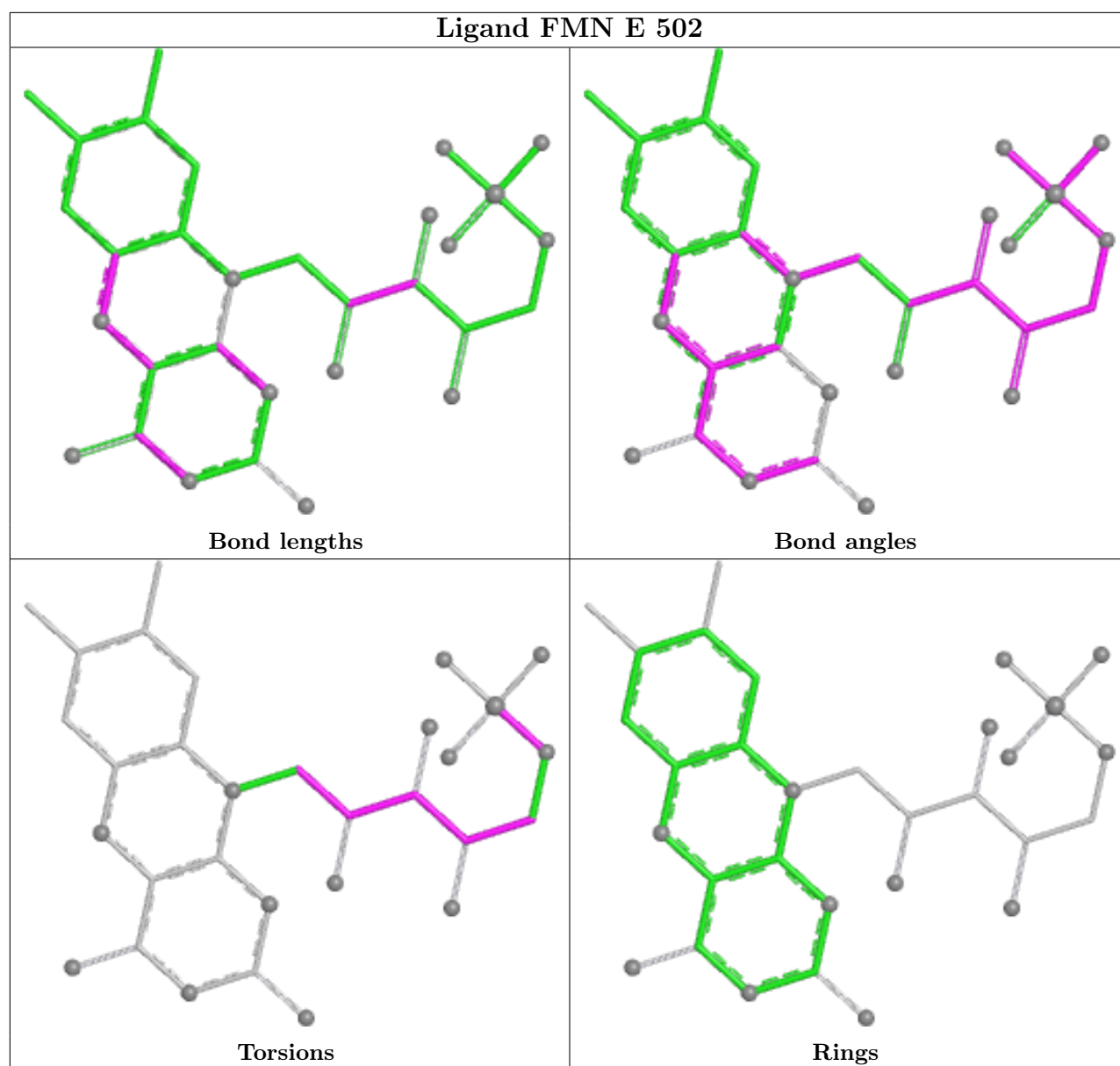
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

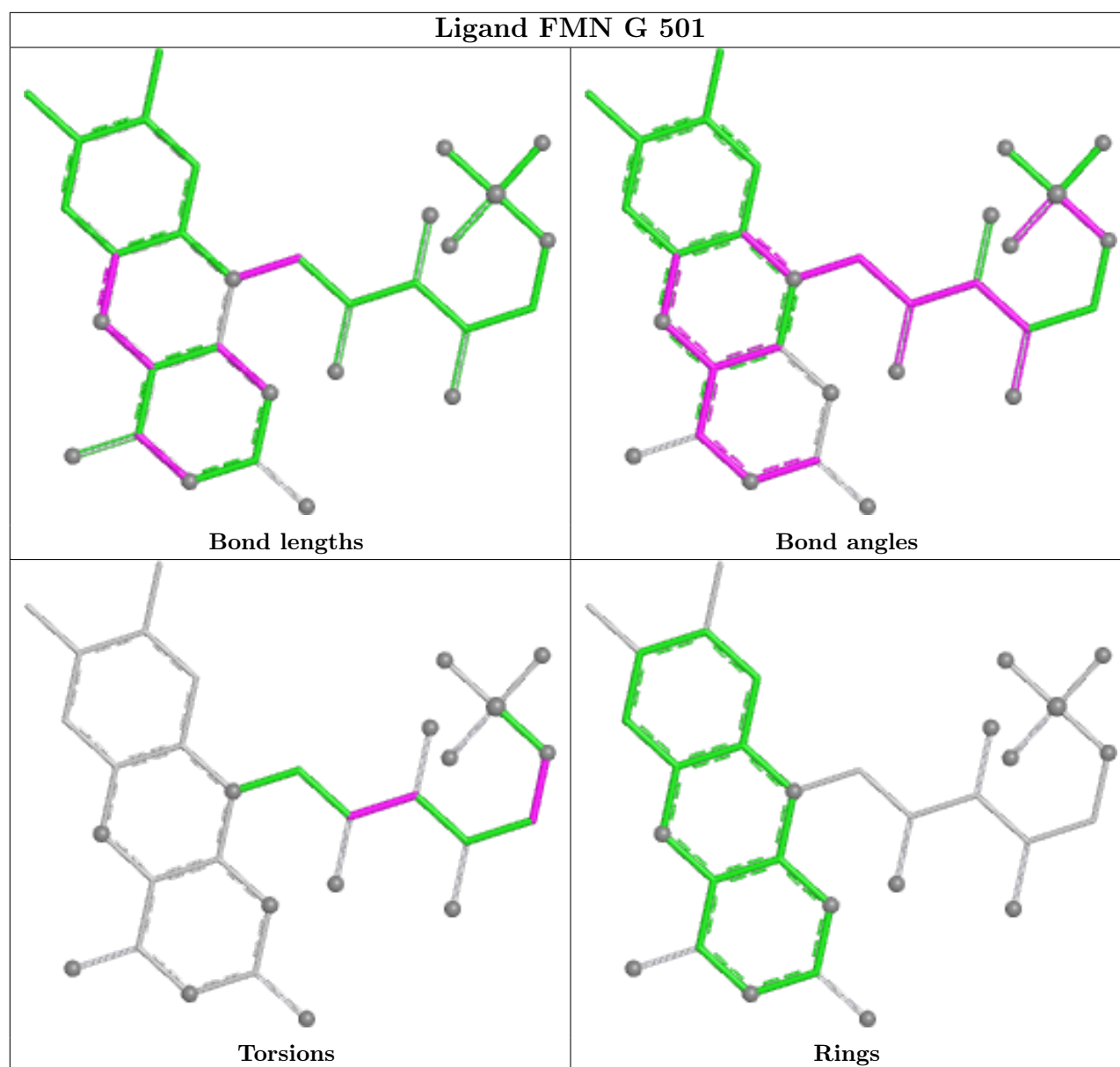
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	B	407/422 (96%)	0.30	14 (3%) 45 35	30, 69, 96, 114	0
1	C	413/422 (97%)	0.22	12 (2%) 51 41	38, 54, 80, 96	0
1	E	409/422 (96%)	0.70	48 (11%) 4 2	55, 74, 98, 120	0
1	G	407/422 (96%)	0.93	65 (15%) 1 1	30, 86, 127, 148	0
All	All	1636/1688 (96%)	0.54	139 (8%) 10 5	30, 71, 108, 148	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	406	GLY	4.7
1	G	229	TYR	4.7
1	G	150	LEU	4.3
1	G	280	THR	4.3
1	G	231	ASN	4.3
1	G	215	HIS	4.1
1	E	151	ASN	4.1
1	E	405	ARG	3.8
1	E	8	PRO	3.8
1	B	28	ASN	3.8
1	G	169	GLY	3.8
1	E	349	ASP	3.7
1	C	159	ASN	3.7
1	G	211	PHE	3.6
1	G	134	GLN	3.5
1	G	177	GLU	3.4
1	G	282	THR	3.4
1	G	212	ILE	3.3
1	E	281	GLU	3.3
1	C	183	ARG	3.3
1	G	220	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	174	PRO	3.3
1	G	210	ASP	3.3
1	G	86	GLY	3.3
1	G	279	SER	3.3
1	E	183	ARG	3.3
1	G	132	GLY	3.2
1	E	218	HIS	3.2
1	E	267	LEU	3.2
1	C	160	VAL	3.1
1	E	217	ALA	3.1
1	G	136	ALA	3.1
1	B	154	SER	3.1
1	E	177	GLU	3.1
1	E	215	HIS	3.0
1	G	88	ILE	3.0
1	G	234	THR	3.0
1	E	230	ALA	3.0
1	G	133	ILE	3.0
1	C	181	ARG	2.9
1	E	275	LEU	2.9
1	G	237	TYR	2.9
1	E	214	ILE	2.9
1	G	172	ASP	2.9
1	E	344	VAL	2.9
1	G	160	VAL	2.9
1	C	270	SER	2.9
1	G	199	ALA	2.8
1	E	312	HIS	2.8
1	G	171	SER	2.8
1	G	178	THR	2.8
1	B	183	ARG	2.8
1	E	372	GLN	2.8
1	E	229	TYR	2.8
1	E	4	ILE	2.8
1	E	334	ALA	2.8
1	B	228	PRO	2.7
1	E	368	GLY	2.7
1	E	28	ASN	2.7
1	G	217	ALA	2.7
1	B	4	ILE	2.7
1	E	316	GLU	2.7
1	E	264	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	268	ARG	2.7
1	B	178	THR	2.6
1	E	57	SER	2.6
1	G	402	GLN	2.5
1	G	313	SER	2.5
1	C	187	GLN	2.5
1	G	31	THR	2.5
1	G	189	ASP	2.5
1	G	214	ILE	2.5
1	G	312	HIS	2.5
1	B	159	ASN	2.5
1	G	213	GLU	2.4
1	B	231	ASN	2.4
1	G	170	PRO	2.4
1	E	135	LEU	2.4
1	E	242	GLU	2.4
1	G	218	HIS	2.4
1	E	58	PRO	2.4
1	E	239	GLY	2.4
1	G	89	MET	2.4
1	G	185	MET	2.4
1	G	32	SER	2.4
1	G	87	LEU	2.4
1	C	56	VAL	2.4
1	E	220	TYR	2.3
1	E	412	PRO	2.3
1	G	130	LYS	2.3
1	E	7	GLU	2.3
1	B	345	GLY	2.3
1	G	241	PHE	2.3
1	E	34	LYS	2.3
1	C	58	PRO	2.3
1	G	33	GLY	2.3
1	G	79	GLY	2.3
1	E	59	MET	2.3
1	B	186	THR	2.2
1	G	270	SER	2.2
1	G	4	ILE	2.2
1	G	173	ILE	2.2
1	G	216	ASN	2.2
1	E	35	ALA	2.2
1	G	337	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	134	GLN	2.2
1	C	28	ASN	2.2
1	G	243	ASN	2.2
1	G	209	ALA	2.2
1	E	181	ARG	2.2
1	E	269	LEU	2.2
1	G	102	SER	2.1
1	C	269	LEU	2.1
1	E	150	LEU	2.1
1	E	88	ILE	2.1
1	G	358	GLU	2.1
1	E	276	GLY	2.1
1	B	158	GLU	2.1
1	B	151	ASN	2.1
1	E	280	THR	2.1
1	E	333	LYS	2.1
1	G	190	ILE	2.1
1	G	281	GLU	2.1
1	C	220	TYR	2.1
1	E	184	ALA	2.1
1	G	34	LYS	2.1
1	G	167	VAL	2.1
1	G	414	VAL	2.1
1	C	134	GLN	2.1
1	G	262	HIS	2.1
1	G	187	GLN	2.1
1	E	172	ASP	2.1
1	B	276	GLY	2.1
1	E	3	ASP	2.0
1	G	90	ILE	2.0
1	G	183	ARG	2.0
1	G	191	ARG	2.0
1	G	85	PRO	2.0
1	G	168	LYS	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 [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

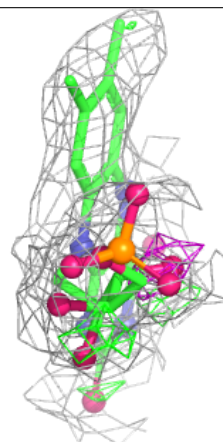
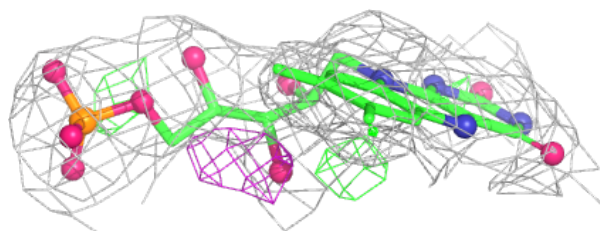
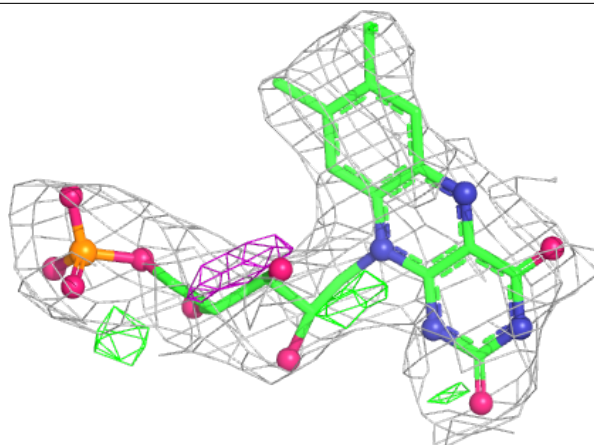
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MPD	E	501	8/8	0.78	0.29	75,78,80,81	0
2	SO4	C	501	5/5	0.84	0.68	48,49,49,51	5
2	SO4	E	503	5/5	0.85	0.64	33,33,33,33	5
2	SO4	B	501	5/5	0.88	0.57	55,55,56,58	5
3	FMN	E	502	31/31	0.89	0.35	33,33,33,33	0
3	FMN	B	502	31/31	0.90	0.33	33,33,33,33	0
2	SO4	G	502	5/5	0.92	0.27	33,33,33,33	5
3	FMN	C	502	31/31	0.92	0.32	33,33,33,33	0
3	FMN	G	501	31/31	0.94	0.16	33,33,33,33	0

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.



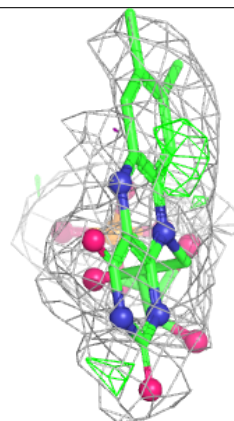
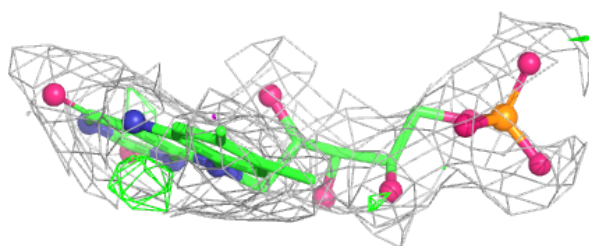
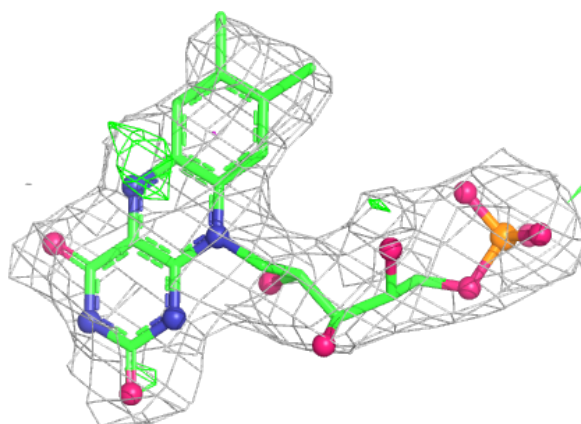
**Electron density around FMN E 502:**

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



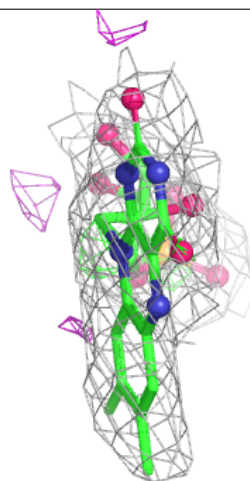
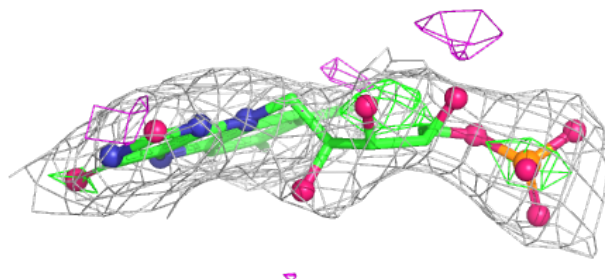
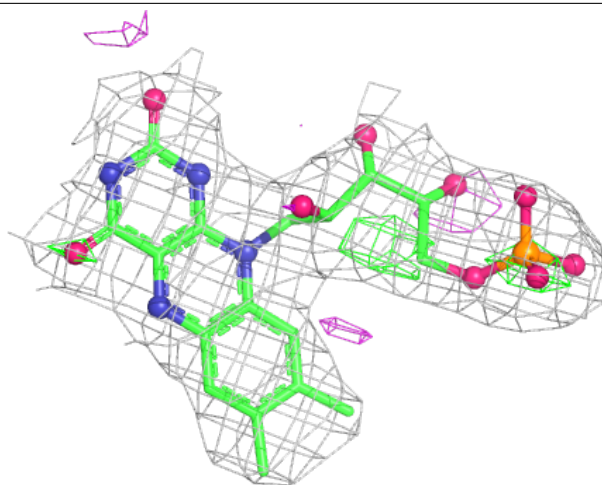
**Electron density around FMN B 502:**

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



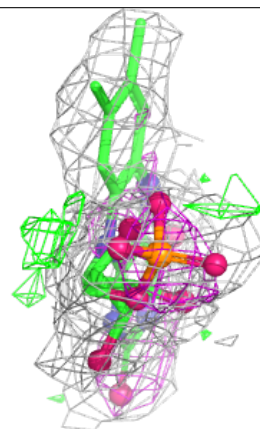
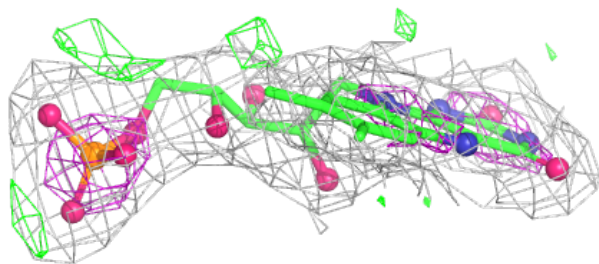
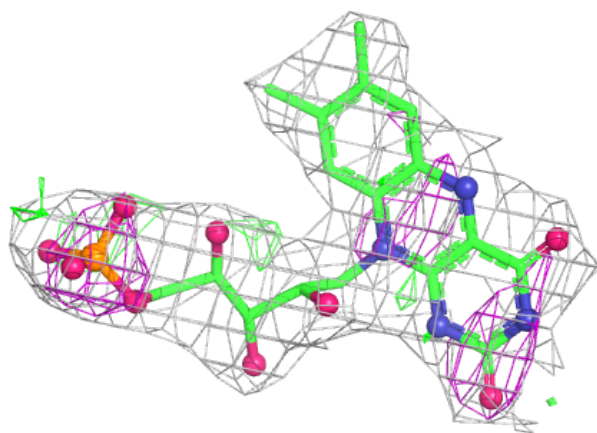
**Electron density around FMN C 502:**

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



**Electron density around FMN G 501:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.