



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2024 – 12:23 AM EST

PDB ID : 4QAI  
Title : P. stipitis OYE2.6-Y78W  
Authors : Sullivan, B.; Walton, A.Z.; Stewart, J.D.  
Deposited on : 2014-05-05  
Resolution : 2.75 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.

The types of validation reports are described at

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

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

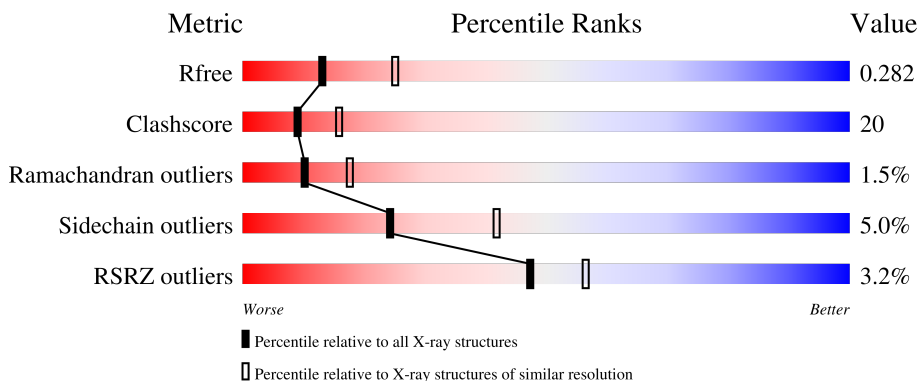
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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.



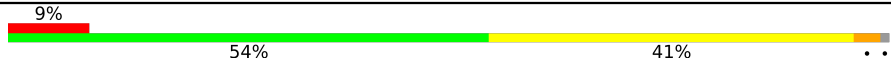
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	A	407	 69% 29% ..
1	B	407	 73% 26% .
1	C	407	 69% 28% ..
1	D	407	 52% 42% 5% .
1	E	407	 64% 33% ..

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Mol	Chain	Length	Quality of chain
1	F	407	

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	FMN	E	501	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19422 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.

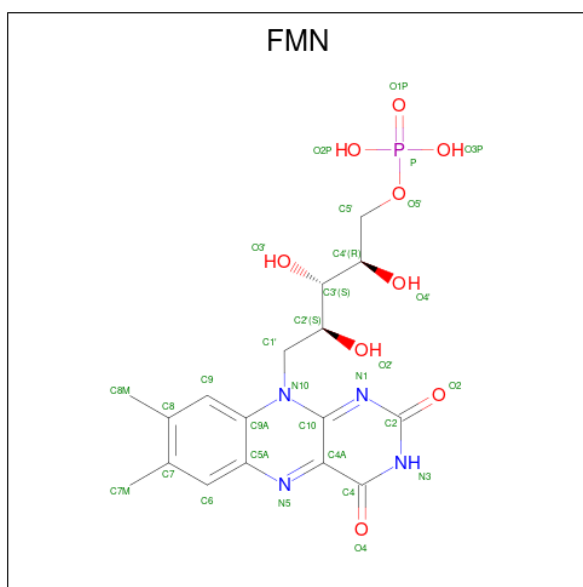
- Molecule 1 is a protein called NADPH dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	404	3203	2029	539	630	5	0	6	0
1	B	404	3203	2029	539	630	5	0	6	0
1	C	404	3203	2029	539	630	5	0	6	0
1	D	404	3201	2027	539	630	5	0	6	0
1	E	404	3201	2028	539	629	5	0	6	0
1	F	404	3203	2029	539	630	5	0	6	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	TRP	TYR	engineered mutation	UNP A3LT82
A	169	ALA	THR	conflict	UNP A3LT82
B	78	TRP	TYR	engineered mutation	UNP A3LT82
B	169	ALA	THR	conflict	UNP A3LT82
C	78	TRP	TYR	engineered mutation	UNP A3LT82
C	169	ALA	THR	conflict	UNP A3LT82
D	78	TRP	TYR	engineered mutation	UNP A3LT82
D	169	ALA	THR	conflict	UNP A3LT82
E	78	TRP	TYR	engineered mutation	UNP A3LT82
E	169	ALA	THR	conflict	UNP A3LT82
F	78	TRP	TYR	engineered mutation	UNP A3LT82
F	169	ALA	THR	conflict	UNP A3LT82

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

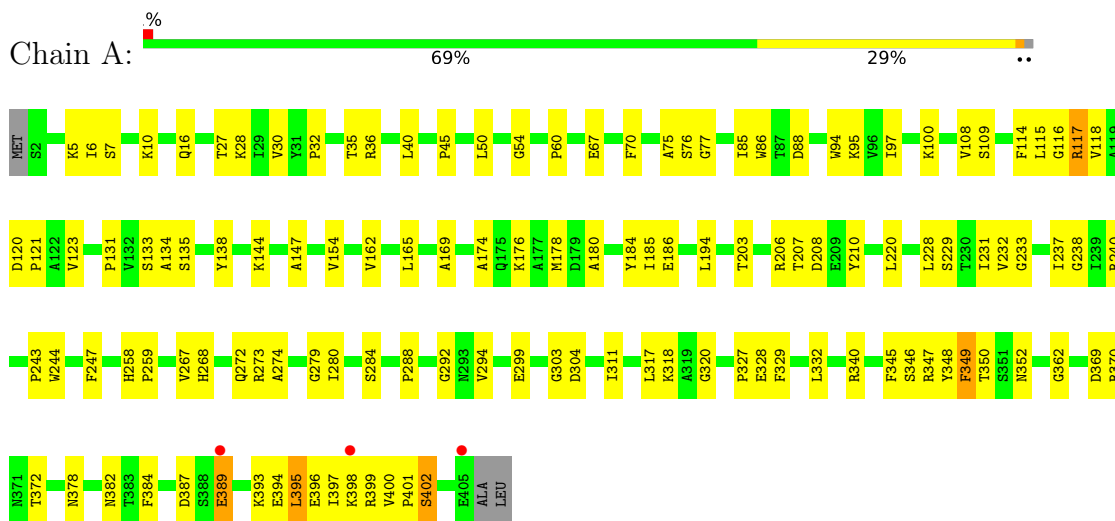
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	5	Total	O	0	0
			5	5		
3	C	2	Total	O	0	0
			2	2		
3	D	3	Total	O	0	0
			3	3		
3	E	5	Total	O	0	0
			5	5		

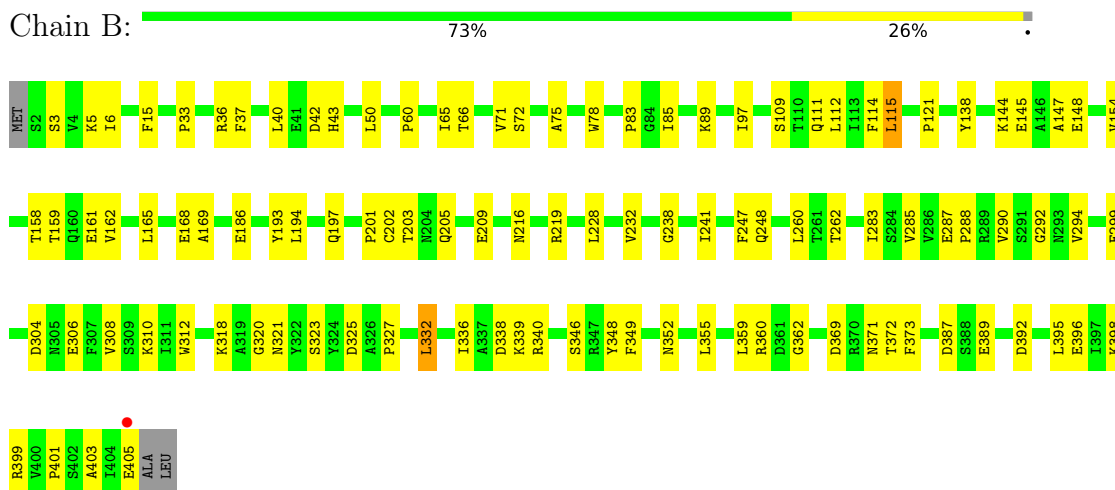
### 3 Residue-property plots [i](#)

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: NADPH dehydrogenase

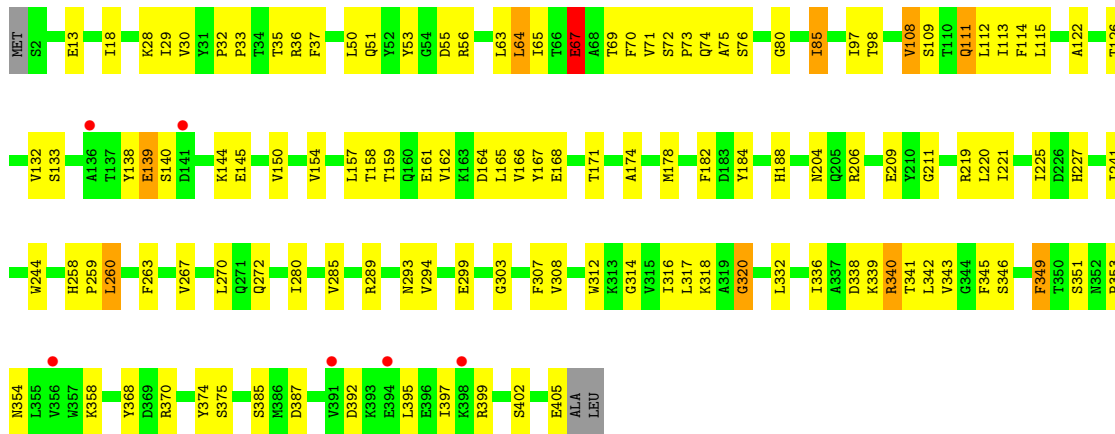


- Molecule 1: NADPH dehydrogenase

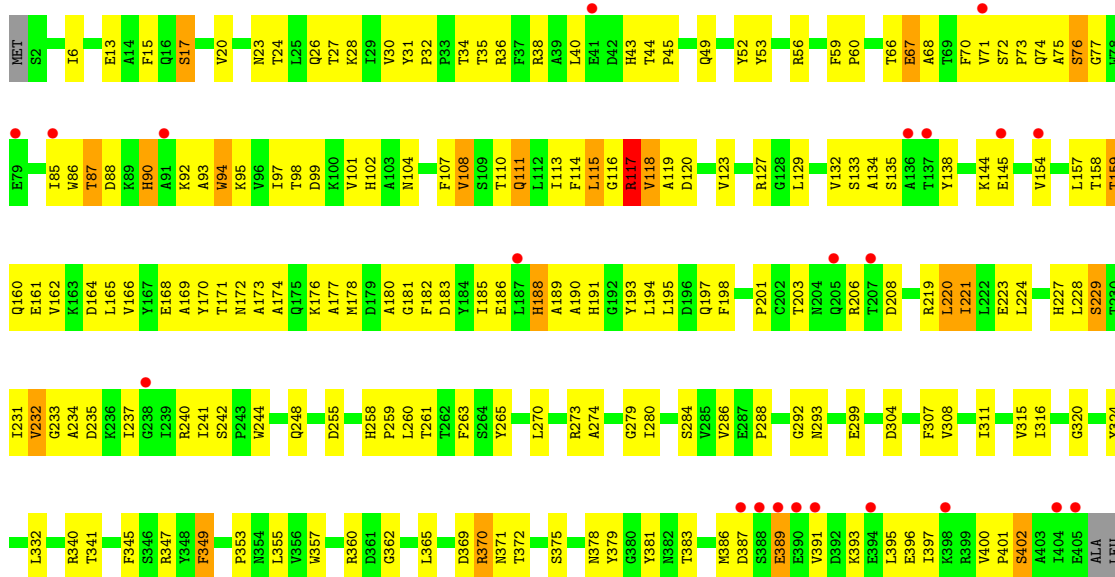


- Molecule 1: NADPH dehydrogenase

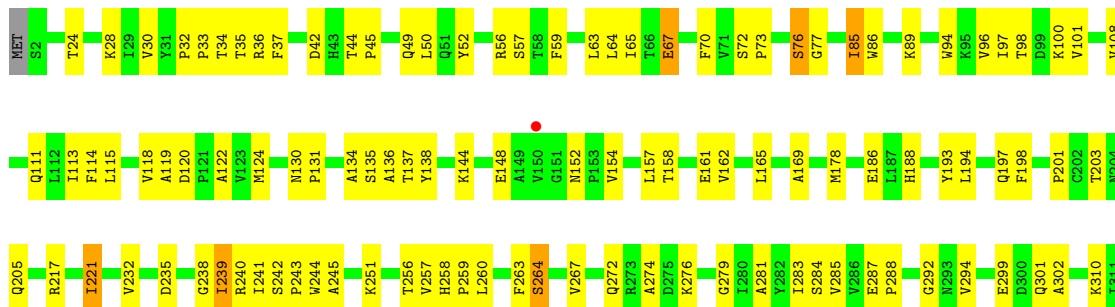


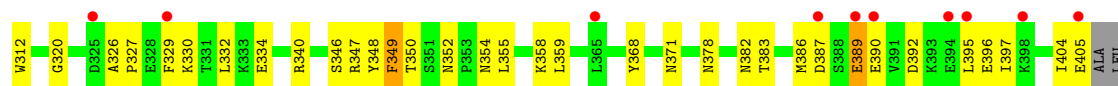


• Molecule 1: NADPH dehydrogenase

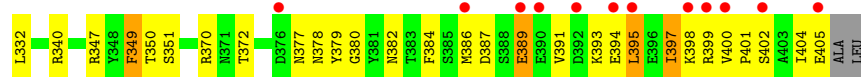
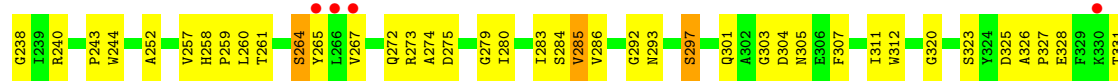


• Molecule 1: NADPH dehydrogenase





● Molecule 1: NADPH dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	226.79Å 226.79Å 360.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.65 – 2.75 48.65 – 2.75	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.65-2.75) 95.4 (48.65-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.73Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.224 , 0.280 0.226 , 0.282	Depositor DCC
$R_{free}$ test set	2000 reflections (2.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.2	Xtrriage
Anisotropy	0.306	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 34.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19422	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.0916e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: 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	A	0.49	0/3293	0.62	0/4476
1	B	0.50	0/3293	0.65	0/4476
1	C	0.47	0/3293	0.62	0/4476
1	D	0.47	0/3293	0.63	0/4476
1	E	0.47	0/3293	0.59	0/4476
1	F	0.45	0/3293	0.57	0/4476
All	All	0.47	0/19758	0.61	0/26856

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	F	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	F	3	SER	Peptide

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

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3203	0	3130	102	0
1	B	3203	0	3130	66	0
1	C	3203	0	3130	86	0
1	D	3201	0	3126	200	0
1	E	3201	0	3130	123	0
1	F	3203	0	3130	201	0
2	A	31	0	19	5	0
2	B	31	0	19	3	0
2	C	31	0	19	3	0
2	D	31	0	19	5	0
2	E	31	0	19	11	0
2	F	31	0	19	6	0
3	A	7	0	0	1	0
3	B	5	0	0	2	0
3	C	2	0	0	1	0
3	D	3	0	0	2	0
3	E	5	0	0	3	0
All	All	19422	0	18890	771	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 20.

All (771) 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:E:347:ARG:NH2	2:E:501:FMN:O2P	1.80	1.13
1:A:399:ARG:HG3	1:A:399:ARG:HH11	1.16	1.11
1:F:393:LYS:HG2	1:F:397:ILE:HD11	1.26	1.11
1:A:346:SER:HB3	2:A:501:FMN:O3P	1.55	1.06
1:F:125:LYS:O	1:F:128:GLY:N	1.88	1.06
1:F:162:VAL:HG11	1:F:210:TYR:CD2	1.91	1.04
1:D:293:ASN:O	1:D:370:ARG:NH2	1.91	1.03
1:E:33:PRO:HD3	1:E:65:ILE:HG21	1.41	1.01
1:A:162:VAL:HG11	1:A:210:TYR:CE2	1.97	0.99
1:D:171:THR:HG23	1:D:231:ILE:CD1	1.95	0.95
1:C:293:ASN:O	1:C:370:ARG:NH2	1.99	0.95
1:D:171:THR:HG23	1:D:231:ILE:HD13	1.49	0.94
1:E:138:TYR:CZ	1:E:154:VAL:HG12	2.01	0.94
1:D:166:VAL:HG21	1:D:223:GLU:OE1	1.66	0.94
1:F:267:VAL:HG12	1:F:311:ILE:HG22	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:TYR:CZ	1:B:154:VAL:HG12	2.05	0.92
1:E:33:PRO:HD3	1:E:65:ILE:CG2	1.99	0.91
1:D:70:PHE:CE1	1:D:76:SER:HA	2.04	0.91
1:A:394[A]:GLU:HG2	1:A:398:LYS:HE2	1.53	0.91
1:F:117:ARG:NH1	1:F:203:THR:HG22	1.85	0.91
1:F:40:LEU:HD21	1:F:402:SER:O	1.70	0.90
1:F:293:ASN:O	1:F:370:ARG:NH2	2.04	0.90
1:F:393:LYS:O	1:F:397:ILE:HG12	1.71	0.90
1:D:228:LEU:O	1:D:232:VAL:HG23	1.72	0.89
1:F:186:GLU:HA	1:F:238:GLY:O	1.72	0.89
1:D:273:ARG:HG3	1:D:273:ARG:HH11	1.38	0.89
1:B:287:GLU:OE2	1:B:318:LYS:NZ	2.07	0.87
1:A:393:LYS:O	1:A:397:ILE:HG13	1.76	0.86
1:F:404:ILE:HG22	1:F:405:GLU:HG3	1.54	0.86
1:D:221:ILE:HD12	1:D:221:ILE:H	1.39	0.86
1:F:162:VAL:HG11	1:F:210:TYR:HD2	1.37	0.86
1:D:120:ASP:OD1	1:D:123:VAL:HG23	1.75	0.86
1:D:117:ARG:NH1	1:D:203:THR:HG22	1.92	0.85
1:D:258:HIS:CD2	1:F:311:ILE:HG12	2.12	0.84
1:D:378:ASN:ND2	1:D:396:GLU:OE1	2.09	0.83
1:B:346:SER:N	2:B:501:FMN:O1P	2.11	0.83
1:F:393:LYS:CG	1:F:397:ILE:HD11	2.09	0.83
1:D:270:LEU:HD22	1:D:280:ILE:HD13	1.61	0.82
1:A:117:ARG:NH1	1:A:203:THR:HG22	1.95	0.82
1:F:40:LEU:HD23	1:F:401:PRO:HB2	1.59	0.82
1:D:116:GLY:O	1:D:118:VAL:N	2.12	0.81
1:C:162:VAL:O	1:C:165:LEU:HB2	1.81	0.81
1:D:117:ARG:HB3	1:D:197:GLN:OE1	1.80	0.81
1:A:162:VAL:HG11	1:A:210:TYR:CD2	2.16	0.81
1:C:317:LEU:HD12	1:C:318:LYS:N	1.95	0.80
1:F:162:VAL:CG1	1:F:210:TYR:CE2	2.65	0.80
1:F:215:GLU:OE1	1:F:215:GLU:N	2.13	0.79
1:A:162:VAL:CG1	1:A:210:TYR:CE2	2.66	0.79
1:D:74:GLN:O	1:D:74:GLN:HG3	1.82	0.79
1:F:267:VAL:HG12	1:F:311:ILE:CG2	2.12	0.79
1:A:138:TYR:CZ	1:A:154:VAL:HG12	2.19	0.78
1:C:332:LEU:C	1:C:332:LEU:HD23	2.04	0.78
1:E:263:PHE:O	1:E:267:VAL:HG23	1.84	0.78
1:A:399:ARG:HG3	1:A:399:ARG:NH1	1.94	0.77
1:A:70:PHE:CE1	1:A:76:SER:HA	2.21	0.76
1:D:162:VAL:HA	1:D:165:LEU:HD12	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HD21	1:A:402:SER:O	1.85	0.76
1:F:114:PHE:CG	1:F:194:LEU:HD22	2.20	0.76
1:E:221:ILE:N	1:E:221:ILE:HD12	2.00	0.76
1:E:135:SER:O	1:E:137:THR:HG23	1.86	0.76
1:D:23:ASN:HB3	1:D:107:PHE:CE1	2.21	0.76
1:D:87:THR:HG23	1:D:90:HIS:CE1	2.20	0.76
1:E:260:LEU:O	1:E:264:SER:OG	2.03	0.76
1:D:31:TYR:HB2	1:D:349:PHE:CE2	2.21	0.75
1:D:134:ALA:O	1:D:206:ARG:CG	2.34	0.75
1:D:311:ILE:HG12	1:F:258:HIS:CD2	2.22	0.75
1:A:138:TYR:CD2	1:A:144:LYS:HB2	2.21	0.75
1:F:132:VAL:HB	1:F:157:LEU:HD21	1.68	0.75
1:A:399:ARG:HH11	1:A:399:ARG:CG	1.98	0.75
1:D:72:SER:HB2	1:D:73:PRO:CD	2.16	0.74
1:D:115:LEU:N	1:D:115:LEU:HD23	2.02	0.74
1:F:73:PRO:HB3	1:F:127:ARG:NH1	2.02	0.74
1:D:165:LEU:HA	1:D:169:ALA:HB3	1.70	0.74
1:D:248:GLN:NE2	3:D:603:HOH:O	2.10	0.73
1:F:244:TRP:CH2	1:F:303:GLY:HA3	2.24	0.73
1:F:273:ARG:HG3	1:F:273:ARG:HH11	1.54	0.73
1:D:273:ARG:HG3	1:D:273:ARG:NH1	2.04	0.72
1:A:114:PHE:CD1	1:A:194:LEU:HD22	2.24	0.72
1:F:74:GLN:HG3	1:F:114:PHE:HZ	1.53	0.72
1:A:273:ARG:HG3	1:A:273:ARG:HH11	1.54	0.72
1:F:125:LYS:O	1:F:127:ARG:N	2.22	0.72
1:F:117:ARG:CZ	1:F:203:THR:HG22	2.19	0.72
1:E:221:ILE:HD12	1:E:221:ILE:H	1.55	0.72
1:E:326:ALA:HB1	1:E:327:PRO:HA	1.71	0.71
1:F:237:ILE:HB	1:F:280:ILE:HG22	1.72	0.71
1:B:387:ASP:HB3	1:B:389[A]:GLU:OE1	1.90	0.70
1:C:35:THR:O	1:C:36:ARG:HD2	1.90	0.70
1:C:64:LEU:N	1:C:64:LEU:HD23	2.06	0.70
1:D:221:ILE:HD12	1:D:221:ILE:N	2.06	0.70
1:A:75:ALA:HB2	1:A:114:PHE:CD2	2.26	0.70
1:A:138:TYR:CG	1:A:144:LYS:HB2	2.27	0.70
1:D:59:PHE:HD2	1:D:357:TRP:CH2	2.10	0.70
1:F:86:TRP:CD1	1:F:87:THR:HG23	2.26	0.70
1:D:224:LEU:O	1:D:228:LEU:HD12	1.91	0.69
1:F:162:VAL:CG1	1:F:210:TYR:CD2	2.71	0.69
1:F:199:LEU:HD21	1:F:221:ILE:HG12	1.73	0.69
1:E:65:ILE:HD13	3:E:604:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:GLU:O	1:F:151:GLY:N	2.23	0.69
1:F:144:LYS:HE3	1:F:148:GLU:OE2	1.93	0.69
1:D:220:LEU:HD11	1:D:224:LEU:HD11	1.73	0.69
1:D:40:LEU:HD23	1:D:401:PRO:HB2	1.74	0.69
1:D:72:SER:HB2	1:D:73:PRO:HD2	1.74	0.69
1:F:283:ILE:HD12	1:F:312:TRP:CG	2.28	0.69
1:C:71:VAL:HG12	1:C:112:LEU:HB3	1.75	0.68
1:D:178:MET:SD	1:D:232:VAL:CG1	2.81	0.68
1:F:395:LEU:HD12	1:F:395:LEU:O	1.94	0.68
1:E:330:LYS:NZ	1:E:334:GLU:OE2	2.26	0.68
1:D:74:GLN:NE2	1:D:132:VAL:HG22	2.08	0.68
1:E:33:PRO:HG2	1:E:240:ARG:NH1	2.08	0.68
1:A:165:LEU:HA	1:A:169:ALA:HB3	1.76	0.68
1:F:274:ALA:HA	1:F:279:GLY:N	2.08	0.67
1:B:325:ASP:OD1	3:B:604:HOH:O	2.12	0.67
1:F:162:VAL:HG11	1:F:210:TYR:CE2	2.29	0.67
1:F:379:TYR:CE1	1:F:393:LYS:HG3	2.29	0.67
1:D:258:HIS:ND1	1:D:259:PRO:HD2	2.09	0.67
1:D:178:MET:SD	1:D:232:VAL:HG12	2.34	0.67
1:E:158:THR:OG1	1:E:161:GLU:HG3	1.94	0.67
1:D:132:VAL:HB	1:D:157:LEU:HD21	1.76	0.67
1:A:27:THR:HG23	3:A:607:HOH:O	1.94	0.67
1:B:40:LEU:HD23	1:B:401:PRO:HB2	1.76	0.67
1:D:20:VAL:HG22	1:D:315:VAL:HG21	1.76	0.66
1:F:201:PRO:HG3	1:F:257:VAL:HG23	1.77	0.66
1:E:221:ILE:H	1:E:221:ILE:CD1	2.08	0.66
1:A:6:ILE:HD12	1:A:362:GLY:HA2	1.78	0.66
1:D:170:TYR:O	1:D:173:ALA:HB3	1.94	0.66
1:E:56:ARG:HB3	1:E:349:PHE:HE1	1.60	0.66
1:A:120:ASP:OD1	1:A:123:VAL:HG23	1.95	0.66
1:E:56:ARG:HB3	1:E:349:PHE:CE1	2.31	0.66
1:F:132:VAL:CB	1:F:157:LEU:HD21	2.25	0.66
1:D:118:VAL:HG23	1:D:118:VAL:O	1.96	0.65
1:E:387:ASP:HB3	1:E:389[A]:GLU:HG3	1.78	0.65
1:A:320:GLY:HA2	2:A:501:FMN:C5'	2.27	0.65
1:D:393:LYS:O	1:D:397:ILE:HG12	1.96	0.65
1:B:336:ILE:O	3:B:603:HOH:O	2.14	0.64
1:F:50:LEU:HD13	1:F:97:ILE:HG13	1.79	0.64
1:D:31:TYR:OH	1:D:34:THR:HB	1.97	0.64
1:A:378:ASN:CB	1:A:399:ARG:HD2	2.27	0.64
1:D:221:ILE:HA	1:D:224:LEU:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:229:SER:HA	1:F:237:ILE:HD11	1.79	0.64
1:D:220:LEU:O	1:D:220:LEU:HD12	1.98	0.64
1:D:270:LEU:HD22	1:D:280:ILE:CD1	2.27	0.64
1:F:74:GLN:HG3	1:F:114:PHE:CZ	2.32	0.64
1:D:174:ALA:HB2	1:D:228:LEU:HD22	1.80	0.64
1:E:355:LEU:HG	1:E:359:LEU:HD12	1.78	0.63
1:F:132:VAL:HB	1:F:157:LEU:CD2	2.27	0.63
1:F:178:MET:SD	1:F:232:VAL:HG12	2.37	0.63
1:B:158:THR:OG1	1:B:161:GLU:HG3	1.98	0.63
1:D:186:GLU:OE2	1:D:240:ARG:HB2	1.98	0.63
1:F:30:VAL:HG13	1:F:63:LEU:O	1.98	0.63
1:F:186:GLU:OE2	1:F:240:ARG:HB2	1.97	0.63
1:F:162:VAL:HG12	1:F:210:TYR:CE2	2.33	0.63
1:D:35:THR:HA	1:D:67:GLU:HB2	1.81	0.63
1:D:201:PRO:HG2	1:D:255:ASP:OD1	1.98	0.63
1:F:75:ALA:HB1	1:F:114:PHE:HA	1.80	0.63
1:F:33:PRO:HG2	1:F:240:ARG:HH11	1.64	0.62
2:D:501:FMN:H2'	2:D:501:FMN:H9	1.80	0.62
1:F:159:THR:O	1:F:159:THR:HG22	1.99	0.62
1:F:243:PRO:O	1:F:259:PRO:HB3	2.00	0.62
1:F:328:GLU:OE2	1:F:328:GLU:HA	2.00	0.62
1:A:60:PRO:HB2	1:B:60:PRO:HB2	1.81	0.62
1:D:113:ILE:HD11	1:D:193:TYR:CE2	2.35	0.62
1:E:348:TYR:O	1:E:352:ASN:HB2	1.99	0.61
1:D:134:ALA:O	1:D:206:ARG:HG3	1.99	0.61
1:F:138:TYR:CD1	1:F:144:LYS:HA	2.36	0.61
1:B:288:PRO:HG3	1:B:304:ASP:HA	1.82	0.61
1:D:221:ILE:H	1:D:221:ILE:CD1	2.11	0.61
1:E:33:PRO:HG2	1:E:240:ARG:HH11	1.65	0.61
1:A:77:GLY:HA3	1:A:115:LEU:HD12	1.81	0.61
1:C:18:ILE:HG21	1:C:342:LEU:HD21	1.81	0.61
1:E:283:ILE:HG22	1:E:285:VAL:HG13	1.83	0.61
1:E:354:ASN:OD1	1:E:358:LYS:HE3	2.01	0.61
1:F:399:ARG:HG3	1:F:399:ARG:HH11	1.64	0.61
1:D:15:PHE:CE1	1:D:360:ARG:HD2	2.36	0.61
1:E:35:THR:H	2:E:501:FMN:C6	2.14	0.61
1:A:317:LEU:HD12	1:A:318:LYS:N	2.16	0.60
1:E:346:SER:HB3	2:E:501:FMN:O3P	2.00	0.60
1:E:35:THR:N	2:E:501:FMN:H6	2.16	0.60
1:D:345:PHE:O	1:D:349:PHE:HB2	2.01	0.60
1:F:133:SER:OG	1:F:134:ALA:N	2.24	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:320:GLY:HA2	2:F:501:FMN:H5'1	1.83	0.60
1:B:114:PHE:CD1	1:B:194:LEU:HD22	2.37	0.60
1:C:241:ILE:HG13	1:C:285:VAL:HG12	1.84	0.60
1:E:347:ARG:CZ	2:E:501:FMN:O2P	2.50	0.60
1:B:42:ASP:OD2	1:B:89:LYS:NZ	2.27	0.60
1:B:396:GLU:OE1	1:B:396:GLU:HA	2.02	0.59
1:E:221:ILE:N	1:E:221:ILE:CD1	2.65	0.59
1:F:109:SER:HB2	1:F:184:TYR:HB2	1.82	0.59
1:B:247:PHE:CD2	1:B:248:GLN:HG3	2.38	0.59
1:D:101:VAL:HG11	1:D:108:VAL:HG12	1.82	0.59
1:E:378:ASN:OD1	1:E:382:ASN:HB2	2.02	0.59
1:F:240:ARG:HA	1:F:284:SER:O	2.02	0.59
1:A:75:ALA:HB2	1:A:114:PHE:CE2	2.37	0.59
1:B:332:LEU:HD23	1:B:332:LEU:C	2.22	0.59
1:F:56:ARG:HB3	1:F:349:PHE:CE1	2.37	0.59
1:D:52:TYR:CE1	1:D:56:ARG:CZ	2.85	0.59
1:D:68:ALA:HB1	1:D:113:ILE:HB	1.85	0.59
1:E:347:ARG:HB3	1:E:368:TYR:CD2	2.38	0.59
1:D:270:LEU:CD2	1:D:280:ILE:HD13	2.33	0.59
1:F:285:VAL:HG23	1:F:305:ASN:ND2	2.18	0.59
1:D:70:PHE:CZ	1:D:76:SER:HA	2.36	0.59
1:D:174:ALA:HB2	1:D:228:LEU:CD2	2.33	0.59
1:D:75:ALA:HB2	1:D:114:PHE:CE2	2.37	0.58
1:F:114:PHE:CD1	1:F:194:LEU:HD22	2.37	0.58
1:F:234:ALA:HA	1:F:237:ILE:HD12	1.86	0.58
1:E:162:VAL:O	1:E:165:LEU:HB2	2.02	0.58
1:D:75:ALA:HB2	1:D:114:PHE:CD2	2.38	0.58
1:D:241:ILE:HD12	1:D:263:PHE:HD1	1.67	0.58
1:D:166:VAL:O	1:D:171:THR:OG1	2.21	0.58
1:E:347:ARG:O	1:E:350:THR:OG1	2.15	0.58
1:D:164:ASP:O	1:D:168:GLU:HB2	2.04	0.58
1:F:148:GLU:O	1:F:150:VAL:N	2.37	0.58
1:C:138:TYR:CD2	1:C:144:LYS:HB2	2.38	0.58
1:A:77:GLY:CA	1:A:115:LEU:HD12	2.34	0.57
1:C:30:VAL:O	1:C:32:PRO:HD3	2.04	0.57
1:D:158:THR:O	1:D:161:GLU:N	2.37	0.57
1:F:116:GLY:O	1:F:118:VAL:N	2.37	0.57
1:C:56:ARG:HG2	1:C:349:PHE:CE1	2.39	0.57
1:C:346:SER:HB3	2:C:501:FMN:O3P	2.04	0.57
1:D:227:HIS:NE2	1:D:231:ILE:HD11	2.19	0.57
1:F:285:VAL:HG23	1:F:305:ASN:HD22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ILE:O	1:A:280:ILE:HB	2.04	0.57
1:C:33:PRO:HG3	1:C:111:GLN:NE2	2.19	0.57
1:E:65:ILE:CD1	3:E:604:HOH:O	2.52	0.57
1:F:35:THR:H	2:F:501:FMN:H6	1.68	0.57
1:A:6:ILE:CD1	1:A:362:GLY:HA2	2.35	0.57
1:C:272:GLN:HE22	1:E:256:THR:HA	1.70	0.57
1:C:317:LEU:HD12	1:C:318:LYS:H	1.70	0.57
1:D:110:THR:HB	1:D:182:PHE:CE1	2.40	0.57
1:F:404:ILE:O	1:F:405:GLU:HB2	2.05	0.57
1:B:6:ILE:HG13	1:B:362:GLY:HA2	1.87	0.57
1:B:33:PRO:HD3	1:B:65:ILE:HB	1.86	0.56
1:B:71:VAL:HG12	1:B:112:LEU:HB3	1.87	0.56
1:A:378:ASN:HB2	1:A:399:ARG:HD2	1.87	0.56
1:A:220:LEU:HD12	1:A:220:LEU:O	2.04	0.56
1:A:400:VAL:HB	1:A:401:PRO:HD2	1.85	0.56
1:C:70:PHE:CE1	1:C:76:SER:HA	2.39	0.56
1:D:59:PHE:CD2	1:D:357:TRP:CH2	2.91	0.56
1:E:73:PRO:O	1:E:76:SER:OG	2.23	0.56
1:F:131:PRO:O	1:F:154:VAL:HA	2.04	0.56
1:B:355:LEU:HG	1:B:359:LEU:HD12	1.85	0.56
1:E:36:ARG:O	1:E:37:PHE:HB2	2.05	0.56
1:E:59:PHE:CD1	1:E:59:PHE:C	2.79	0.56
1:A:121:PRO:HG3	1:A:147:ALA:HA	1.87	0.56
1:D:40:LEU:HD21	1:D:402:SER:O	2.06	0.56
1:D:265:TYR:HB2	1:F:261:THR:HG21	1.86	0.56
1:E:70:PHE:HB2	1:E:86:TRP:HZ3	1.71	0.56
1:F:36:ARG:NH2	1:F:380:GLY:O	2.35	0.56
1:F:78:TRP:CE2	1:F:115:LEU:HD11	2.40	0.56
1:F:244:TRP:CZ2	1:F:303:GLY:HA3	2.41	0.56
1:F:33:PRO:HG2	1:F:240:ARG:NH1	2.21	0.56
1:F:95:LYS:HA	1:F:180:ALA:O	2.06	0.56
1:F:178:MET:CG	1:F:232:VAL:HG12	2.35	0.56
1:A:186:GLU:HA	1:A:238:GLY:O	2.04	0.56
1:D:133:SER:OG	1:D:135:SER:O	2.23	0.56
1:F:70:PHE:HB2	1:F:86:TRP:HZ3	1.70	0.56
1:A:40:LEU:HD23	1:A:401:PRO:HB2	1.87	0.56
1:A:320:GLY:HA2	2:A:501:FMN:H5'1	1.86	0.56
2:D:501:FMN:H2'	2:D:501:FMN:C9	2.36	0.56
1:E:50:LEU:HD11	1:E:100:LYS:HD2	1.87	0.56
1:E:138:TYR:CE1	1:E:154:VAL:HG12	2.39	0.56
1:C:338:ASP:O	1:C:339:LYS:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:ARG:HA	1:E:284:SER:O	2.05	0.56
1:F:326:ALA:HB1	1:F:327:PRO:HA	1.88	0.56
1:C:74:GLN:O	1:C:74:GLN:HG3	2.05	0.55
1:E:49:GLN:NE2	1:E:67:GLU:OE2	2.34	0.55
1:F:114:PHE:CG	1:F:194:LEU:CD2	2.90	0.55
1:C:72:SER:HB2	1:C:73:PRO:HD2	1.88	0.55
1:D:31:TYR:HB2	1:D:349:PHE:CD2	2.41	0.55
1:F:260:LEU:O	1:F:264:SER:OG	2.18	0.55
1:D:75:ALA:CB	1:D:114:PHE:CD2	2.89	0.55
1:F:159:THR:OG1	1:F:208:ASP:OD2	2.23	0.55
1:D:308:VAL:HG12	1:D:316:ILE:HD13	1.89	0.55
1:F:34:THR:O	1:F:67:GLU:HB3	2.06	0.55
1:F:351:SER:O	1:F:384:PHE:HB3	2.07	0.55
1:C:108:VAL:HG22	1:C:182:PHE:HD1	1.71	0.55
1:E:396:GLU:OE1	1:E:396:GLU:HA	2.05	0.55
1:F:40:LEU:CD2	1:F:401:PRO:HB2	2.33	0.55
1:F:45:PRO:HA	1:F:49:GLN:OE1	2.06	0.55
1:F:285:VAL:CG2	1:F:305:ASN:ND2	2.70	0.55
1:C:138:TYR:CZ	1:C:154:VAL:HG12	2.42	0.55
1:E:243:PRO:HB2	1:E:244:TRP:CD1	2.41	0.55
1:D:59:PHE:HD2	1:D:357:TRP:CZ2	2.25	0.55
1:D:274:ALA:HA	1:D:279:GLY:CA	2.37	0.55
1:E:52:TYR:O	1:E:56:ARG:NH1	2.39	0.55
1:D:93:ALA:C	1:D:95:LYS:H	2.09	0.54
1:A:400:VAL:HB	1:A:401:PRO:CD	2.37	0.54
1:B:33:PRO:HD3	1:B:65:ILE:CG2	2.36	0.54
1:F:75:ALA:O	1:F:115:LEU:HD23	2.07	0.54
1:F:229:SER:HA	1:F:237:ILE:CD1	2.37	0.54
1:A:369:ASP:OD2	1:A:372:THR:HG23	2.06	0.54
1:C:53:TYR:OH	1:C:67:GLU:OE2	2.21	0.54
1:D:307:PHE:HB2	1:F:260:LEU:HD13	1.89	0.54
1:E:258:HIS:ND1	1:E:260:LEU:HB2	2.23	0.54
1:D:94:TRP:HA	1:D:97:ILE:HD12	1.88	0.54
1:D:133:SER:OG	1:D:134:ALA:N	2.35	0.54
1:F:40:LEU:HD23	1:F:401:PRO:CB	2.34	0.54
1:C:69:THR:HG22	1:C:85:ILE:HG22	1.90	0.54
1:A:274:ALA:HA	1:A:279:GLY:N	2.23	0.54
1:C:164:ASP:O	1:C:168:GLU:HB2	2.08	0.54
1:C:392:ASP:OD2	1:C:395:LEU:HB2	2.07	0.54
1:D:102:HIS:C	1:D:104:ASN:H	2.11	0.54
1:D:117:ARG:HG2	1:D:118:VAL:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ILE:HG13	1:B:285:VAL:HG12	1.90	0.54
1:D:171:THR:CG2	1:D:231:ILE:HD13	2.33	0.54
1:E:329:PHE:HB3	1:E:332:LEU:HB3	1.90	0.54
1:F:162:VAL:CG1	1:F:210:TYR:HE2	2.17	0.54
1:A:109:SER:HB2	1:A:184:TYR:HB2	1.89	0.53
1:D:383:THR:O	1:D:386:MET:HG3	2.08	0.53
1:F:74:GLN:OE1	1:F:129:LEU:HD22	2.08	0.53
1:F:75:ALA:HA	1:F:114:PHE:CD1	2.43	0.53
1:B:75:ALA:HB1	1:B:114:PHE:HA	1.90	0.53
1:D:70:PHE:CD1	1:D:76:SER:HA	2.41	0.53
1:D:332:LEU:HD23	1:D:332:LEU:C	2.28	0.53
1:E:50:LEU:HA	1:E:97:ILE:HG12	1.91	0.53
1:A:117:ARG:O	1:A:117:ARG:HG3	2.09	0.53
1:E:33:PRO:CD	1:E:65:ILE:HG21	2.29	0.53
1:F:33:PRO:HD3	1:F:65:ILE:HG21	1.90	0.53
1:F:226:ASP:O	1:F:230:THR:HG23	2.08	0.53
1:F:252:ALA:O	1:F:259:PRO:HD3	2.08	0.53
1:F:229:SER:O	1:F:233:GLY:HA2	2.08	0.53
1:B:158:THR:O	1:B:159:THR:C	2.46	0.53
1:B:306:GLU:HG3	1:B:310:LYS:HE2	1.90	0.53
1:C:13:GLU:O	1:C:28:LYS:HD2	2.09	0.53
1:D:241:ILE:HD12	1:D:263:PHE:CD1	2.43	0.53
1:D:400:VAL:HB	1:D:401:PRO:CD	2.39	0.53
1:F:158:THR:O	1:F:162:VAL:HG23	2.09	0.53
1:E:135:SER:O	1:E:137:THR:N	2.42	0.53
1:A:399:ARG:NH1	1:A:399:ARG:CG	2.62	0.52
1:F:88:ASP:OD1	1:F:176:LYS:HE3	2.09	0.52
1:B:50:LEU:HA	1:B:97:ILE:HG12	1.91	0.52
1:E:35:THR:H	2:E:501:FMN:C5A	2.22	0.52
1:E:114:PHE:CD1	1:E:194:LEU:HD22	2.45	0.52
1:F:33:PRO:HD3	1:F:65:ILE:CG2	2.40	0.52
1:F:285:VAL:CG2	1:F:305:ASN:HD22	2.22	0.52
1:A:75:ALA:CB	1:A:114:PHE:CD2	2.93	0.52
1:A:332:LEU:C	1:A:332:LEU:HD23	2.29	0.52
1:C:111:GLN:OE1	1:C:188:HIS:CD2	2.63	0.52
1:E:389[B]:GLU:HG2	1:E:390:GLU:N	2.25	0.52
1:F:320:GLY:HA2	2:F:501:FMN:C5'	2.39	0.52
1:C:221:ILE:HD12	1:C:221:ILE:N	2.25	0.52
1:D:158:THR:O	1:D:160:GLN:N	2.43	0.52
1:F:283:ILE:HD12	1:F:312:TRP:CD1	2.44	0.52
1:C:332:LEU:C	1:C:332:LEU:CD2	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:VAL:HG12	1:C:316:ILE:CD1	2.40	0.52
1:D:74:GLN:HE21	1:D:132:VAL:HG22	1.75	0.52
1:A:174:ALA:O	1:A:178:MET:HG2	2.10	0.51
1:E:30:VAL:HG13	1:E:63:LEU:O	2.10	0.51
1:E:35:THR:H	2:E:501:FMN:H6	1.72	0.51
1:E:44:THR:HG22	1:E:45:PRO:HD2	1.92	0.51
1:E:392:ASP:OD2	1:E:395:LEU:HB2	2.10	0.51
1:D:237:ILE:O	1:D:280:ILE:HB	2.10	0.51
1:E:33:PRO:HD3	1:E:65:ILE:CB	2.39	0.51
2:A:501:FMN:O3P	2:A:501:FMN:O4'	2.26	0.51
1:E:77:GLY:HA3	1:E:119:ALA:HB1	1.93	0.51
1:E:287:GLU:OE1	1:E:288:PRO:HD2	2.10	0.51
1:F:273:ARG:HG3	1:F:273:ARG:NH1	2.24	0.51
1:A:267:VAL:HG12	1:A:311:ILE:HG22	1.93	0.51
1:A:347:ARG:O	1:A:350:THR:OG1	2.18	0.51
1:B:78:TRP:CE2	1:B:115:LEU:HD11	2.46	0.51
1:B:392:ASP:OD2	1:B:395:LEU:HB2	2.11	0.51
1:C:108:VAL:HG22	1:C:182:PHE:CD1	2.45	0.51
1:B:216:ASN:OD1	1:B:219:ARG:NH2	2.42	0.51
1:D:190:ALA:HB1	1:D:242:SER:OG	2.11	0.51
1:D:244:TRP:CZ3	1:D:258:HIS:HE1	2.28	0.51
1:F:163:LYS:HD3	1:F:210:TYR:OH	2.10	0.51
1:F:224:LEU:O	1:F:228:LEU:HB2	2.11	0.51
1:D:242:SER:HB3	1:D:286:VAL:HG21	1.93	0.51
1:C:51:GLN:HG2	1:C:55:ASP:OD2	2.11	0.50
1:C:336:ILE:HG22	1:C:343:VAL:HG13	1.93	0.50
1:D:53:TYR:OH	1:D:66:THR:HA	2.11	0.50
1:A:240:ARG:HA	1:A:284:SER:O	2.11	0.50
1:F:25:LEU:CD2	1:F:107:PHE:CD2	2.94	0.50
1:A:16:GLN:O	1:A:28:LYS:NZ	2.45	0.50
1:D:240:ARG:HA	1:D:284:SER:O	2.12	0.50
1:E:217:ARG:NH2	1:E:257:VAL:HG21	2.26	0.50
1:F:159:THR:O	1:F:159:THR:CG2	2.59	0.50
1:F:399:ARG:HG3	1:F:399:ARG:NH1	2.26	0.50
1:C:139:GLU:HG2	1:C:140:SER:N	2.27	0.50
1:E:64:LEU:O	1:E:108:VAL:HA	2.12	0.50
1:A:185:ILE:HG13	1:A:185:ILE:O	2.11	0.50
1:B:247:PHE:CD1	1:B:292:GLY:HA3	2.47	0.50
1:C:33:PRO:HG2	2:C:501:FMN:C2	2.42	0.50
1:C:397:ILE:HG22	1:C:397:ILE:O	2.11	0.50
1:D:28:LYS:HD3	1:D:341:THR:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:THR:OG1	1:D:181:GLY:HA3	2.11	0.50
1:D:157:LEU:O	1:D:206:ARG:NH1	2.45	0.50
1:E:113:ILE:HG12	1:E:114:PHE:N	2.27	0.50
1:F:304:ASP:OD2	1:F:304:ASP:N	2.43	0.50
1:E:397:ILE:HG22	1:E:397:ILE:O	2.11	0.50
1:A:70:PHE:CD1	1:A:76:SER:HA	2.46	0.50
1:A:178:MET:CG	1:A:232:VAL:HG12	2.41	0.50
1:E:194:LEU:O	1:E:197:GLN:HB2	2.11	0.50
1:E:347:ARG:HD2	1:E:368:TYR:CZ	2.47	0.50
1:F:78:TRP:NE1	1:F:115:LEU:HD11	2.27	0.50
1:F:394[A]:GLU:HG2	1:F:398:LYS:CE	2.41	0.50
1:A:5:LYS:O	1:A:327:PRO:HB3	2.12	0.50
1:E:96:VAL:HG11	1:E:404:ILE:HG21	1.94	0.50
1:E:404:ILE:O	1:E:405:GLU:HB2	2.11	0.50
1:F:132:VAL:CG2	1:F:157:LEU:HD21	2.42	0.50
1:A:328:GLU:O	1:A:329:PHE:HB2	2.12	0.49
1:C:50:LEU:HA	1:C:97:ILE:HG12	1.93	0.49
1:E:35:THR:N	2:E:501:FMN:C6	2.75	0.49
1:A:86:TRP:O	1:A:176:LYS:HE2	2.12	0.49
1:A:178:MET:HA	1:A:178:MET:CE	2.42	0.49
1:A:273:ARG:HG3	1:A:273:ARG:NH1	2.25	0.49
1:D:72:SER:HA	1:D:86:TRP:CE3	2.47	0.49
1:E:387:ASP:HB3	1:E:389[B]:GLU:OE1	2.12	0.49
1:F:117:ARG:O	1:F:117:ARG:HG3	2.10	0.49
1:D:229:SER:HA	1:D:237:ILE:HD11	1.93	0.49
1:A:378:ASN:OD1	1:A:382:ASN:HB2	2.12	0.49
1:C:113:ILE:HG12	1:C:114:PHE:N	2.27	0.49
1:C:289:ARG:NH2	1:C:320:GLY:O	2.42	0.49
1:D:132:VAL:CB	1:D:157:LEU:HD21	2.43	0.49
1:F:378:ASN:HD22	1:F:399:ARG:HD2	1.76	0.49
1:B:71:VAL:O	1:B:72:SER:HB3	2.12	0.49
1:D:102:HIS:C	1:D:104:ASN:N	2.66	0.49
1:C:71:VAL:CG1	1:C:112:LEU:HB3	2.40	0.49
1:D:260:LEU:CD1	1:F:307:PHE:HB2	2.42	0.49
1:E:34:THR:O	1:E:67:GLU:HB3	2.13	0.49
1:E:50:LEU:HD13	1:E:97:ILE:HA	1.95	0.49
1:C:72:SER:O	1:C:75:ALA:HB3	2.13	0.49
1:D:116:GLY:CA	1:D:132:VAL:O	2.61	0.49
1:C:318:LYS:HD2	1:C:341:THR:CG2	2.43	0.48
1:D:88:ASP:OD1	1:D:176:LYS:HE3	2.13	0.48
1:D:110:THR:HB	1:D:182:PHE:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:TYR:CZ	1:D:154:VAL:HG12	2.48	0.48
1:D:229:SER:O	1:D:233:GLY:HA2	2.13	0.48
1:E:120:ASP:OD1	1:E:122:ALA:HB3	2.13	0.48
1:F:134:ALA:HB2	1:F:198:PHE:CE1	2.49	0.48
1:D:273:ARG:NH1	1:D:273:ARG:CG	2.76	0.48
1:D:30:VAL:O	1:D:32:PRO:HD3	2.13	0.48
1:E:138:TYR:CE2	1:E:154:VAL:HG12	2.46	0.48
1:A:387:ASP:HB3	1:A:389[A]:GLU:OE2	2.13	0.48
1:B:66:THR:HG23	1:B:109:SER:O	2.13	0.48
1:D:52:TYR:CD1	1:D:56:ARG:NH1	2.81	0.48
1:C:308:VAL:HG12	1:C:316:ILE:HD13	1.94	0.48
1:D:185:ILE:HG13	1:D:185:ILE:O	2.13	0.48
1:E:94:TRP:O	1:E:98:THR:HG23	2.14	0.48
1:E:186:GLU:HA	1:E:238:GLY:O	2.13	0.48
1:F:148:GLU:C	1:F:150:VAL:H	2.17	0.48
1:A:178:MET:SD	1:A:232:VAL:HG12	2.54	0.48
1:A:394[A]:GLU:CG	1:A:398:LYS:HE2	2.35	0.48
1:D:400:VAL:HB	1:D:401:PRO:HD2	1.96	0.48
1:F:76:SER:OG	1:F:77:GLY:N	2.46	0.48
1:F:85:ILE:HG23	1:F:173:ALA:HB1	1.96	0.48
1:F:204:ASN:OD1	1:F:204:ASN:C	2.52	0.48
1:F:379:TYR:HB2	1:F:397:ILE:HD13	1.94	0.48
1:F:372:THR:HG21	1:F:379:TYR:CD2	2.49	0.48
1:D:45:PRO:HG3	1:D:94:TRP:CE2	2.48	0.48
1:C:244:TRP:CH2	1:C:303:GLY:HA3	2.48	0.47
1:D:308:VAL:HG12	1:D:316:ILE:CD1	2.44	0.47
1:A:178:MET:HA	1:A:178:MET:HE2	1.95	0.47
1:C:37:PHE:CG	1:C:80:GLY:HA3	2.49	0.47
1:D:117:ARG:O	1:D:117:ARG:HG3	2.13	0.47
1:F:274:ALA:HB2	1:F:279:GLY:HA3	1.95	0.47
1:B:395:LEU:O	1:B:398:LYS:HB2	2.15	0.47
1:C:259:PRO:O	1:C:263:PHE:HD2	1.97	0.47
1:D:40:LEU:CD2	1:D:401:PRO:HB2	2.44	0.47
1:F:43:HIS:HD2	1:F:86:TRP:HH2	1.63	0.47
1:B:348:TYR:O	1:B:352:ASN:HB2	2.15	0.47
1:E:201:PRO:HG3	1:E:257:VAL:HG23	1.95	0.47
1:A:288:PRO:HG3	1:A:304:ASP:HA	1.97	0.47
1:C:206:ARG:HB2	1:C:211:GLY:HA3	1.96	0.47
1:D:93:ALA:C	1:D:95:LYS:N	2.66	0.47
1:D:138:TYR:CE2	1:D:144:LYS:HG3	2.50	0.47
1:F:191:HIS:CE1	1:F:292:GLY:HA2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LEU:HD12	1:A:317:LEU:C	2.34	0.47
1:D:66:THR:OG1	1:D:110:THR:HA	2.15	0.47
1:F:155:ARG:HH22	1:F:161:GLU:CD	2.18	0.47
1:F:378:ASN:ND2	1:F:399:ARG:HD2	2.30	0.47
1:F:393:LYS:O	1:F:397:ILE:CG1	2.55	0.47
1:A:88:ASP:OD1	1:A:176:LYS:HE3	2.15	0.47
1:B:5:LYS:O	1:B:327:PRO:HB3	2.15	0.47
1:B:144:LYS:O	1:B:148:GLU:HG3	2.14	0.47
1:C:332:LEU:HD23	1:C:332:LEU:O	2.14	0.47
1:C:354:ASN:OD1	1:C:358:LYS:HE3	2.15	0.47
1:C:374:TYR:CZ	2:C:501:FMN:HM72	2.49	0.47
1:D:114:PHE:HD1	1:D:194:LEU:HB2	1.80	0.47
1:D:160:GLN:NE2	1:D:164:ASP:OD1	2.46	0.47
1:E:114:PHE:CG	1:E:194:LEU:HD22	2.49	0.47
1:F:272:GLN:HA	1:F:275:ASP:OD2	2.14	0.47
1:A:348:TYR:O	1:A:352:ASN:HB2	2.15	0.47
1:F:274:ALA:CB	1:F:279:GLY:HA3	2.45	0.47
1:A:138:TYR:CD1	1:A:144:LYS:HA	2.50	0.47
1:D:23:ASN:CB	1:D:107:PHE:CE1	2.97	0.47
1:D:134:ALA:O	1:D:206:ARG:HG2	2.13	0.47
1:E:36:ARG:NH1	1:E:350:THR:HG22	2.30	0.47
1:F:75:ALA:HB2	1:F:114:PHE:CD2	2.50	0.47
1:F:56:ARG:HG3	1:F:56:ARG:HH11	1.79	0.46
1:C:263:PHE:O	1:C:267:VAL:HG23	2.16	0.46
1:E:242:SER:HB2	1:E:245:ALA:HB2	1.98	0.46
1:F:347:ARG:O	1:F:350:THR:OG1	2.20	0.46
1:E:272:GLN:O	1:E:276:LYS:HG3	2.15	0.46
1:F:115:LEU:N	1:F:115:LEU:CD2	2.79	0.46
1:F:178:MET:SD	1:F:232:VAL:CG1	3.04	0.46
1:F:221:ILE:CD1	1:F:221:ILE:N	2.79	0.46
1:A:50:LEU:HA	1:A:97:ILE:HG12	1.96	0.46
1:C:336:ILE:HA	1:C:341:THR:HB	1.97	0.46
1:D:72:SER:CB	1:D:73:PRO:CD	2.88	0.46
1:D:102:HIS:NE2	1:D:183:ASP:OD2	2.41	0.46
1:F:201:PRO:HG3	1:F:257:VAL:CG2	2.44	0.46
1:B:33:PRO:HD3	1:B:65:ILE:HG21	1.97	0.46
1:D:70:PHE:CE2	1:D:76:SER:HB2	2.50	0.46
1:D:13:GLU:HG3	1:D:13:GLU:O	2.15	0.46
1:D:17:SER:HB3	1:D:26:GLN:OE1	2.16	0.46
1:D:261:THR:OG1	1:F:264:SER:HB2	2.15	0.46
1:B:186:GLU:HA	1:B:238:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:VAL:O	1:C:171:THR:OG1	2.30	0.46
1:D:158:THR:O	1:D:159:THR:C	2.54	0.46
1:D:220:LEU:CD1	1:D:224:LEU:HD11	2.43	0.46
1:E:201:PRO:O	1:E:205[A]:GLN:NE2	2.45	0.46
1:E:292:GLY:O	2:E:501:FMN:H1'2	2.15	0.46
1:E:288:PRO:O	1:E:301:GLN:HG2	2.15	0.46
1:F:91:ALA:HA	1:F:180:ALA:HB2	1.97	0.46
1:C:353:PRO:HG3	1:C:385[B]:SER:OG	2.16	0.46
1:D:6:ILE:HG13	1:D:362:GLY:HA2	1.97	0.46
1:E:144:LYS:HE2	1:E:148:GLU:OE2	2.16	0.46
1:F:237:ILE:O	1:F:280:ILE:HB	2.15	0.46
1:C:260:LEU:HD21	1:C:307:PHE:CG	2.51	0.45
1:D:45:PRO:HG2	1:D:94:TRP:CD1	2.51	0.45
1:F:35:THR:H	2:F:501:FMN:C6	2.29	0.45
1:F:325:ASP:OD2	1:F:331:THR:HB	2.15	0.45
1:F:5:LYS:O	1:F:327:PRO:HB3	2.15	0.45
1:A:346:SER:HB3	2:A:501:FMN:HO4'	1.81	0.45
1:E:30:VAL:HG22	1:E:63:LEU:HB3	1.98	0.45
1:F:69:THR:HG23	1:F:83:PRO:O	2.17	0.45
1:B:33:PRO:HD3	1:B:65:ILE:CB	2.46	0.45
1:B:228:LEU:O	1:B:232:VAL:HG22	2.16	0.45
1:F:25:LEU:HD23	1:F:107:PHE:CE2	2.50	0.45
1:F:351:SER:HA	1:F:384:PHE:CG	2.52	0.45
1:B:209:GLU:H	1:B:209:GLU:HG2	1.54	0.45
1:C:29:ILE:O	3:C:601:HOH:O	2.21	0.45
1:D:233:GLY:O	1:D:235:ASP:N	2.50	0.45
1:F:109:SER:CB	1:F:184:TYR:HB2	2.46	0.45
1:F:120:ASP:O	1:F:124:MET:HG2	2.16	0.45
1:F:211:GLY:N	1:F:216:ASN:HB3	2.31	0.45
1:D:74:GLN:O	1:D:74:GLN:CG	2.61	0.45
1:F:98:THR:HG22	1:F:108:VAL:HG11	1.99	0.45
1:F:218:ALA:HB3	1:F:265:TYR:HE1	1.81	0.45
1:D:258:HIS:HD2	1:F:311:ILE:HG12	1.73	0.45
1:F:50:LEU:HA	1:F:97:ILE:HG12	1.98	0.45
1:F:274:ALA:HB2	1:F:279:GLY:CA	2.47	0.45
1:D:23:ASN:HB3	1:D:107:PHE:CZ	2.51	0.45
1:D:52:TYR:HB2	1:D:381:TYR:CE2	2.51	0.45
1:D:162:VAL:O	1:D:165:LEU:HB2	2.17	0.45
1:F:25:LEU:CD2	1:F:107:PHE:HD2	2.28	0.45
1:C:270:LEU:HD22	1:C:280:ILE:HD13	1.98	0.45
1:D:70:PHE:HE1	1:D:115:LEU:HD21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:LEU:O	1:F:232:VAL:HG22	2.17	0.45
1:F:378:ASN:OD1	1:F:382:ASN:HB2	2.16	0.45
1:A:45:PRO:HG2	1:A:94:TRP:CD1	2.51	0.45
1:A:134:ALA:O	1:A:206:ARG:CG	2.65	0.45
1:A:268:HIS:O	1:A:272:GLN:HG3	2.17	0.45
1:D:43:HIS:NE2	1:D:127:ARG:NH2	2.65	0.45
1:F:394[A]:GLU:HG2	1:F:398:LYS:HE3	1.99	0.45
1:C:132:VAL:O	1:C:133:SER:HB2	2.16	0.44
1:D:34:THR:O	1:D:36:ARG:HG2	2.17	0.44
1:D:241:ILE:HB	1:D:263:PHE:CE1	2.52	0.44
1:D:311:ILE:HD11	1:F:260:LEU:HD12	1.99	0.44
1:E:355:LEU:HG	1:E:359:LEU:CD1	2.44	0.44
1:F:43:HIS:CD2	1:F:86:TRP:HH2	2.34	0.44
1:F:117:ARG:CZ	1:F:203:THR:CG2	2.94	0.44
1:F:158:THR:C	1:F:160:GLN:H	2.20	0.44
1:B:65:ILE:HD13	1:B:186:GLU:OE1	2.16	0.44
1:B:40:LEU:HD23	1:B:401:PRO:CB	2.47	0.44
1:B:201:PRO:O	1:B:205[B]:GLN:NE2	2.40	0.44
1:C:318:LYS:HD2	1:C:341:THR:HG21	1.99	0.44
1:C:158:THR:O	1:C:159:THR:C	2.54	0.44
1:C:345:PHE:O	1:C:349:PHE:HB2	2.17	0.44
1:F:240:ARG:HH21	1:F:286:VAL:HG22	1.83	0.44
1:A:30:VAL:O	1:A:32:PRO:HD3	2.17	0.44
1:C:260:LEU:HD21	1:C:307:PHE:CD1	2.52	0.44
1:D:95:LYS:NZ	1:D:99:ASP:OD2	2.44	0.44
1:F:35:THR:N	2:F:501:FMN:H6	2.32	0.44
1:F:260:LEU:HD23	1:F:260:LEU:HA	1.90	0.44
1:A:10:LYS:O	1:A:10:LYS:HG2	2.18	0.44
1:A:70:PHE:HB2	1:A:86:TRP:HZ3	1.83	0.44
1:D:45:PRO:HA	1:D:49:GLN:OE1	2.18	0.44
1:D:71:VAL:O	1:D:86:TRP:HB3	2.17	0.44
1:D:190:ALA:HB2	1:D:241:ILE:HA	1.98	0.44
1:E:131:PRO:HB2	1:E:154:VAL:HB	2.00	0.44
1:F:73:PRO:HB3	1:F:127:ARG:HH11	1.78	0.44
1:C:174:ALA:O	1:C:178:MET:HG2	2.18	0.44
1:D:70:PHE:HB2	1:D:86:TRP:HZ3	1.83	0.44
1:A:247:PHE:CD1	1:A:292:GLY:HA3	2.53	0.44
1:D:191:HIS:CE1	1:D:292:GLY:HA2	2.53	0.44
1:E:251:LYS:HD3	1:E:251:LYS:HA	1.81	0.44
1:C:314:GLY:O	1:C:340:ARG:HD3	2.17	0.44
1:C:351:SER:HB3	1:C:368:TYR:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:VAL:O	1:B:165:LEU:HB2	2.18	0.43
1:B:399:ARG:HG3	1:B:399:ARG:HH11	1.83	0.43
1:C:317:LEU:HD12	1:C:317:LEU:C	2.38	0.43
1:D:198:PHE:CG	1:D:220:LEU:HD23	2.53	0.43
1:F:25:LEU:HD23	1:F:107:PHE:CD2	2.53	0.43
1:F:195:LEU:HB3	1:F:221:ILE:HD11	2.00	0.43
1:A:54:GLY:HA3	1:A:100:LYS:HD3	2.00	0.43
1:A:288:PRO:HG3	1:A:303:GLY:O	2.19	0.43
1:D:116:GLY:C	1:D:118:VAL:H	2.19	0.43
1:D:117:ARG:HG2	1:D:118:VAL:CG1	2.48	0.43
1:F:274:ALA:HA	1:F:279:GLY:CA	2.48	0.43
1:A:45:PRO:HG3	1:A:94:TRP:CE2	2.53	0.43
1:B:197:GLN:HA	1:B:203:THR:OG1	2.18	0.43
1:D:189:ALA:HA	1:D:195:LEU:HB2	1.99	0.43
1:A:131:PRO:HB2	1:A:154:VAL:HA	2.00	0.43
1:A:258:HIS:ND1	1:A:259:PRO:HD2	2.34	0.43
1:D:86:TRP:HB2	1:D:172:ASN:HD21	1.82	0.43
1:D:240:ARG:NH2	2:D:501:FMN:O3'	2.51	0.43
1:A:229:SER:O	1:A:233:GLY:HA2	2.19	0.43
1:B:36:ARG:O	1:B:37:PHE:HB2	2.16	0.43
1:C:98:THR:HG22	1:C:108:VAL:HG11	1.98	0.43
1:C:209:GLU:H	1:C:209:GLU:HG2	1.60	0.43
1:E:130:ASN:HA	1:E:152:ASN:OD1	2.18	0.43
1:E:134:ALA:HB2	1:E:198:PHE:CD1	2.54	0.43
1:A:7[B]:SER:OG	1:A:327:PRO:O	2.26	0.43
1:A:244:TRP:CH2	1:A:303:GLY:HA3	2.53	0.43
1:E:347:ARG:NE	2:E:501:FMN:O2P	2.52	0.43
1:F:125:LYS:O	1:F:126:THR:C	2.57	0.43
1:D:113:ILE:HD11	1:D:193:TYR:CD2	2.53	0.43
1:F:39:ALA:HB3	1:F:81:ALA:O	2.18	0.43
1:F:240:ARG:NH1	2:F:501:FMN:O2'	2.44	0.43
1:C:220:LEU:HD12	1:C:220:LEU:O	2.19	0.43
1:D:6:ILE:HD13	1:D:365:LEU:HD21	2.01	0.43
1:D:118:VAL:O	1:D:118:VAL:CG2	2.65	0.43
1:D:161:GLU:O	1:D:165:LEU:HG	2.19	0.43
1:D:389[A]:GLU:H	1:D:389[A]:GLU:HG3	1.60	0.43
1:E:77:GLY:HA3	1:E:119:ALA:CB	2.47	0.43
1:E:120:ASP:O	1:E:124:MET:HG2	2.19	0.43
1:E:197:GLN:O	1:E:203:THR:OG1	2.14	0.43
1:A:116:GLY:O	1:A:118:VAL:N	2.52	0.43
1:D:369:ASP:OD2	1:D:372:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:SER:HB2	1:E:73:PRO:HD2	2.01	0.43
1:E:85:ILE:HD13	1:E:94:TRP:CD1	2.53	0.43
1:F:70:PHE:CE1	1:F:76:SER:HA	2.53	0.43
1:B:373:PHE:CD2	2:B:501:FMN:HM71	2.54	0.43
1:C:221:ILE:O	1:C:225:ILE:HG12	2.19	0.43
1:D:74:GLN:NE2	1:D:132:VAL:CG2	2.80	0.43
1:D:171:THR:HG23	1:D:231:ILE:HD11	1.92	0.43
1:D:274:ALA:HA	1:D:279:GLY:N	2.34	0.43
1:F:75:ALA:HA	1:F:114:PHE:CE1	2.54	0.43
1:F:165:LEU:O	1:F:170:TYR:HB2	2.19	0.43
1:D:70:PHE:CE2	1:D:76:SER:CB	3.02	0.42
1:E:113:ILE:HD11	1:E:193:TYR:CG	2.54	0.42
1:F:205[B]:GLN:OE1	1:F:205[B]:GLN:HA	2.13	0.42
1:A:114:PHE:CG	1:A:194:LEU:HD22	2.54	0.42
1:F:351:SER:HA	1:F:384:PHE:CD2	2.55	0.42
1:F:372:THR:OG1	1:F:380:GLY:HA3	2.19	0.42
1:D:56:ARG:HG2	1:D:353:PRO:HA	2.00	0.42
1:E:28:LYS:HE2	3:E:603:HOH:O	2.19	0.42
1:F:158:THR:O	1:F:160:GLN:N	2.52	0.42
1:F:210:TYR:CD1	1:F:219:ARG:HD2	2.54	0.42
1:A:243:PRO:HB2	1:A:244:TRP:CD1	2.54	0.42
1:B:285:VAL:HG11	1:B:308:VAL:HG21	2.01	0.42
1:C:204:ASN:OD1	1:C:204:ASN:C	2.58	0.42
1:D:113:ILE:HG12	1:D:114:PHE:N	2.35	0.42
1:E:57:SER:HB2	1:E:101:VAL:HG13	2.01	0.42
1:A:35:THR:O	1:A:36:ARG:HD2	2.18	0.42
1:B:6:ILE:HA	1:B:327:PRO:CB	2.49	0.42
1:B:202:CYS:SG	1:B:203:THR:HG23	2.60	0.42
1:B:320:GLY:O	1:B:321:ASN:C	2.57	0.42
1:D:38:ARG:NH2	1:D:375:SER:OG	2.53	0.42
1:F:132:VAL:HG21	1:F:157:LEU:HD21	2.00	0.42
1:A:396:GLU:HA	1:A:396:GLU:OE1	2.20	0.42
1:C:397:ILE:O	1:C:397:ILE:CG2	2.67	0.42
1:D:24:THR:HG22	1:D:26:GLN:HE22	1.84	0.42
1:D:74:GLN:HB2	1:D:129:LEU:HD13	2.02	0.42
1:F:138:TYR:CE1	1:F:144:LYS:HA	2.54	0.42
1:B:219:ARG:HG3	1:B:219:ARG:HH11	1.84	0.42
1:B:283:ILE:HD12	1:B:312:TRP:CG	2.53	0.42
1:E:157:LEU:HD22	1:E:161:GLU:HB3	2.01	0.42
1:E:241:ILE:HG13	1:E:243:PRO:HD3	2.01	0.42
1:E:274:ALA:HA	1:E:279:GLY:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:PRO:HA	1:F:131:PRO:HG3	2.01	0.42
1:B:121:PRO:HG3	1:B:147:ALA:HA	2.01	0.42
1:F:157:LEU:O	1:F:206:ARG:NH1	2.47	0.42
1:F:297:SER:O	1:F:301:GLN:HG3	2.20	0.42
1:A:228:LEU:O	1:A:232:VAL:HG22	2.20	0.42
1:D:174:ALA:CB	1:D:228:LEU:CD2	2.98	0.42
1:D:195:LEU:HD21	1:D:224:LEU:CD1	2.49	0.42
1:D:260:LEU:HD23	1:D:260:LEU:HA	1.93	0.42
1:E:113:ILE:HG12	1:E:114:PHE:H	1.84	0.42
1:F:400:VAL:HB	1:F:401:PRO:CD	2.50	0.42
1:C:56:ARG:HG2	1:C:349:PHE:CD1	2.54	0.41
1:E:178:MET:SD	1:E:232:VAL:HG12	2.60	0.41
1:E:244:TRP:CZ3	1:E:302:ALA:O	2.73	0.41
1:E:387:ASP:HB3	1:E:389[A]:GLU:CG	2.47	0.41
1:D:59:PHE:HA	1:D:60:PRO:HD3	1.84	0.41
1:F:162:VAL:HG12	1:F:210:TYR:HE2	1.79	0.41
1:F:178:MET:HG3	1:F:232:VAL:HG12	2.01	0.41
1:C:65:ILE:HG12	1:C:109:SER:HB3	2.02	0.41
1:C:258:HIS:HA	1:C:259:PRO:HD3	1.93	0.41
1:D:379:TYR:HB3	1:D:397:ILE:HD13	2.01	0.41
1:E:113:ILE:HD11	1:E:193:TYR:CD2	2.55	0.41
1:E:258:HIS:CE1	1:E:259:PRO:HD2	2.55	0.41
1:F:377:ASN:OD1	1:F:379:TYR:HB3	2.21	0.41
1:F:386:MET:HE2	1:F:391:VAL:HG22	2.02	0.41
1:A:165:LEU:HA	1:A:169:ALA:CB	2.49	0.41
1:D:177:ALA:O	1:D:180:ALA:HB3	2.19	0.41
1:B:369:ASP:O	1:B:371:ASN:N	2.53	0.41
1:C:132:VAL:HB	1:C:157:LEU:HD21	2.01	0.41
1:C:138:TYR:CG	1:C:144:LYS:HB2	2.55	0.41
1:D:77:GLY:HA3	1:D:119:ALA:HB1	2.03	0.41
1:E:30:VAL:O	1:E:32:PRO:HD3	2.19	0.41
1:E:42:ASP:OD2	1:E:89:LYS:NZ	2.35	0.41
1:F:133:SER:O	1:F:157:LEU:HG	2.21	0.41
1:A:133:SER:HB3	1:A:135:SER:O	2.19	0.41
1:A:345:PHE:O	1:A:349:PHE:HB2	2.20	0.41
1:B:323:SER:HG	1:B:348:TYR:HE2	1.68	0.41
1:D:56:ARG:NH1	3:D:602:HOH:O	2.44	0.41
1:D:349:PHE:CE1	1:D:355:LEU:HB3	2.56	0.41
1:E:138:TYR:OH	1:E:154:VAL:N	2.47	0.41
1:F:243:PRO:O	1:F:259:PRO:CB	2.65	0.41
1:C:167:TYR:HD1	1:C:227:HIS:CE1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ARG:HG3	1:C:219:ARG:HH11	1.85	0.41
1:F:216:ASN:O	1:F:217:ARG:C	2.58	0.41
1:B:283:ILE:HD12	1:B:312:TRP:CD2	2.56	0.41
1:B:389[A]:GLU:CD	1:B:389[A]:GLU:H	2.23	0.41
1:E:154:VAL:HG13	1:E:154:VAL:O	2.20	0.41
1:A:95:LYS:HA	1:A:180:ALA:O	2.21	0.41
1:B:138:TYR:OH	1:B:154:VAL:HG12	2.19	0.41
1:B:168:GLU:O	1:B:169:ALA:C	2.58	0.41
1:B:193:TYR:O	1:B:194:LEU:C	2.60	0.41
1:C:122:ALA:O	1:C:126:THR:HG23	2.21	0.41
1:D:92:LYS:O	1:D:95:LYS:HB3	2.21	0.41
1:D:110:THR:HG22	1:D:185:ILE:HG22	2.02	0.41
1:D:111:GLN:OE1	1:D:188:HIS:CD2	2.73	0.41
1:D:244:TRP:HZ3	1:D:258:HIS:HE1	1.68	0.41
1:E:235:ASP:O	1:E:281:ALA:HB2	2.20	0.41
1:F:148:GLU:C	1:F:150:VAL:N	2.73	0.41
1:F:274:ALA:HA	1:F:279:GLY:H	1.82	0.41
1:A:229:SER:HA	1:A:237:ILE:HD11	2.03	0.41
1:B:15:PHE:CZ	1:B:360:ARG:HB2	2.55	0.41
1:B:290:VAL:HG11	2:B:501:FMN:C5'	2.51	0.41
1:D:67:GLU:O	1:D:68:ALA:C	2.59	0.41
1:E:56:ARG:CB	1:E:349:PHE:HE1	2.32	0.41
1:E:59:PHE:HD1	1:E:59:PHE:O	2.04	0.41
1:E:201:PRO:HG3	1:E:257:VAL:CG2	2.51	0.41
1:E:378:ASN:O	1:E:383:THR:HG23	2.20	0.41
1:C:158:THR:O	1:C:161:GLU:N	2.55	0.40
1:D:45:PRO:HG2	1:D:94:TRP:CG	2.57	0.40
1:D:240:ARG:HD3	2:D:501:FMN:O2	2.21	0.40
1:E:346:SER:N	2:E:501:FMN:O3P	2.52	0.40
1:F:332:LEU:C	1:F:332:LEU:HD23	2.41	0.40
1:C:113:ILE:CG1	1:C:114:PHE:N	2.85	0.40
1:D:260:LEU:CD2	1:D:307:PHE:CD1	3.04	0.40
1:D:347:ARG:HG3	2:D:501:FMN:O3P	2.21	0.40
1:E:392:ASP:HB3	1:E:395:LEU:HB3	2.03	0.40
1:F:129:LEU:HD23	1:F:129:LEU:HA	1.90	0.40
1:F:258:HIS:ND1	1:F:259:PRO:HD2	2.36	0.40
1:C:63:LEU:C	1:C:64:LEU:HD23	2.41	0.40
1:C:312:TRP:O	1:C:340:ARG:NH1	2.38	0.40
1:D:219:ARG:O	1:D:223:GLU:HB2	2.22	0.40
1:E:115:LEU:HD12	1:E:118:VAL:HG23	2.03	0.40
1:E:239:ILE:HG13	1:E:240:ARG:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:ALA:HB2	1:F:198:PHE:CD1	2.56	0.40
1:B:43:HIS:O	1:B:83:PRO:HA	2.21	0.40
1:D:288:PRO:HG3	1:D:304:ASP:HA	2.03	0.40
1:A:178:MET:HG3	1:A:232:VAL:HG12	2.03	0.40
1:B:338:ASP:O	1:B:339:LYS:HB2	2.21	0.40
1:C:72:SER:HB2	1:C:73:PRO:CD	2.51	0.40
1:D:59:PHE:CD2	1:D:357:TRP:CZ2	3.08	0.40
1:E:283:ILE:HD12	1:E:312:TRP:CG	2.57	0.40
1:F:20:VAL:O	1:F:20:VAL:HG12	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	408/407 (100%)	371 (91%)	32 (8%)	5 (1%)	13	23
1	B	408/407 (100%)	383 (94%)	23 (6%)	2 (0%)	29	47
1	C	408/407 (100%)	384 (94%)	20 (5%)	4 (1%)	15	27
1	D	408/407 (100%)	356 (87%)	41 (10%)	11 (3%)	5	7
1	E	408/407 (100%)	383 (94%)	20 (5%)	5 (1%)	13	23
1	F	408/407 (100%)	361 (88%)	38 (9%)	9 (2%)	6	11
All	All	2448/2442 (100%)	2238 (91%)	174 (7%)	36 (2%)	10	18

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	85	ILE
1	D	117	ARG
1	E	136	ALA

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Mol	Chain	Res	Type
1	F	117	ARG
1	F	126	THR
1	A	384	PHE
1	A	395	LEU
1	C	67	GLU
1	C	85	ILE
1	D	159	THR
1	D	234	ALA
1	D	391	VAL
1	D	395	LEU
1	F	149	ALA
1	A	117	ARG
1	D	208	ASP
1	E	85	ILE
1	E	169	ALA
1	F	125	LYS
1	F	159	THR
1	F	208	ASP
1	A	208	ASP
1	B	403	ALA
1	C	399	ARG
1	D	76	SER
1	D	90	HIS
1	E	67	GLU
1	F	139	GLU
1	C	320	GLY
1	D	320	GLY
1	E	320	GLY
1	F	90	HIS
1	D	94	TRP
1	D	85	ILE
1	F	221	ILE
1	A	85	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	348/344 (101%)	336 (97%)	12 (3%)	37	58
1	B	348/344 (101%)	335 (96%)	13 (4%)	34	54
1	C	348/344 (101%)	330 (95%)	18 (5%)	23	39
1	D	348/344 (101%)	322 (92%)	26 (8%)	13	23
1	E	348/344 (101%)	332 (95%)	16 (5%)	27	46
1	F	348/344 (101%)	326 (94%)	22 (6%)	18	31
All	All	2088/2064 (101%)	1981 (95%)	107 (5%)	24	41

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	GLU
1	A	108	VAL
1	A	207	THR
1	A	231	ILE
1	A	294	VAL
1	A	299	GLU
1	A	340	ARG
1	A	349	PHE
1	A	370	ARG
1	A	389[A]	GLU
1	A	389[B]	GLU
1	A	402	SER
1	B	3	SER
1	B	111	GLN
1	B	115	LEU
1	B	145	GLU
1	B	260	LEU
1	B	262	THR
1	B	294	VAL
1	B	299	GLU
1	B	332	LEU
1	B	340	ARG
1	B	349	PHE
1	B	372	THR
1	B	405	GLU
1	C	64	LEU
1	C	67	GLU
1	C	108	VAL
1	C	111	GLN
1	C	115	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	139	GLU
1	C	145	GLU
1	C	150	VAL
1	C	184	TYR
1	C	260	LEU
1	C	294	VAL
1	C	299	GLU
1	C	340	ARG
1	C	349	PHE
1	C	375	SER
1	C	387	ASP
1	C	402	SER
1	C	405	GLU
1	D	17	SER
1	D	27	THR
1	D	44	THR
1	D	67	GLU
1	D	87	THR
1	D	108	VAL
1	D	111	GLN
1	D	115	LEU
1	D	117	ARG
1	D	118	VAL
1	D	145	GLU
1	D	188	HIS
1	D	220	LEU
1	D	221	ILE
1	D	229	SER
1	D	232	VAL
1	D	299	GLU
1	D	324	TYR
1	D	340	ARG
1	D	349	PHE
1	D	370	ARG
1	D	371	ASN
1	D	387	ASP
1	D	389[A]	GLU
1	D	389[B]	GLU
1	D	402	SER
1	E	24	THR
1	E	76	SER
1	E	111	GLN

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Mol	Chain	Res	Type
1	E	188	HIS
1	E	221	ILE
1	E	239	ILE
1	E	264	SER
1	E	294	VAL
1	E	299	GLU
1	E	310	LYS
1	E	340	ARG
1	E	349	PHE
1	E	371	ASN
1	E	386	MET
1	E	389[A]	GLU
1	E	389[B]	GLU
1	F	4	VAL
1	F	7[A]	SER
1	F	7[B]	SER
1	F	43	HIS
1	F	111	GLN
1	F	114	PHE
1	F	115	LEU
1	F	117	ARG
1	F	188	HIS
1	F	214	ILE
1	F	221	ILE
1	F	264	SER
1	F	285	VAL
1	F	297	SER
1	F	323	SER
1	F	340	ARG
1	F	349	PHE
1	F	387	ASP
1	F	389[A]	GLU
1	F	389[B]	GLU
1	F	395	LEU
1	F	397	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	272	GLN
1	D	49	GLN
1	D	74	GLN

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Mol	Chain	Res	Type
1	D	90	HIS
1	D	191	HIS
1	D	258	HIS
1	E	248	GLN
1	E	272	GLN
1	F	305	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FMN	E	501	-	33,33,33	1.43	4 (12%)	48,50,50	1.22	6 (12%)
2	FMN	C	501	-	33,33,33	1.43	4 (12%)	48,50,50	1.22	6 (12%)
2	FMN	F	501	-	33,33,33	1.43	4 (12%)	48,50,50	1.21	6 (12%)
2	FMN	B	501	-	33,33,33	1.42	4 (12%)	48,50,50	1.22	6 (12%)
2	FMN	D	501	-	33,33,33	1.43	4 (12%)	48,50,50	1.21	6 (12%)
2	FMN	A	501	-	33,33,33	1.43	4 (12%)	48,50,50	1.22	6 (12%)

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	FMN	E	501	-	-	8/18/18/18	0/3/3/3
2	FMN	C	501	-	-	1/18/18/18	0/3/3/3
2	FMN	F	501	-	-	4/18/18/18	0/3/3/3
2	FMN	B	501	-	-	7/18/18/18	0/3/3/3
2	FMN	D	501	-	-	4/18/18/18	0/3/3/3
2	FMN	A	501	-	-	3/18/18/18	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	FMN	C9A-C5A	5.05	1.49	1.41
2	D	501	FMN	C9A-C5A	5.05	1.49	1.41
2	A	501	FMN	C9A-C5A	5.01	1.49	1.41
2	F	501	FMN	C9A-C5A	5.01	1.49	1.41
2	C	501	FMN	C9A-C5A	5.00	1.49	1.41
2	B	501	FMN	C9A-C5A	4.97	1.49	1.41
2	E	501	FMN	C8-C7	3.32	1.49	1.40
2	F	501	FMN	C8-C7	3.30	1.49	1.40
2	A	501	FMN	C8-C7	3.30	1.49	1.40
2	D	501	FMN	C8-C7	3.30	1.49	1.40
2	B	501	FMN	C8-C7	3.30	1.49	1.40
2	C	501	FMN	C8-C7	3.30	1.49	1.40
2	A	501	FMN	C4A-N5	2.53	1.35	1.30
2	B	501	FMN	C4A-N5	2.52	1.35	1.30
2	D	501	FMN	C4A-N5	2.51	1.35	1.30
2	C	501	FMN	C4A-N5	2.50	1.35	1.30
2	F	501	FMN	C4-N3	-2.49	1.34	1.38
2	C	501	FMN	C4-N3	-2.48	1.34	1.38
2	E	501	FMN	C4-N3	-2.48	1.34	1.38
2	E	501	FMN	C4A-N5	2.47	1.35	1.30
2	F	501	FMN	C4A-N5	2.46	1.35	1.30
2	B	501	FMN	C4-N3	-2.45	1.34	1.38
2	A	501	FMN	C4-N3	-2.45	1.34	1.38
2	D	501	FMN	C4-N3	-2.45	1.34	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	FMN	C4-C4A-N5	2.80	122.22	118.23
2	D	501	FMN	C4-C4A-N5	2.74	122.13	118.23
2	B	501	FMN	C4-C4A-N5	2.73	122.11	118.23
2	A	501	FMN	C4-C4A-N5	2.72	122.10	118.23
2	E	501	FMN	C4-C4A-N5	2.70	122.07	118.23
2	F	501	FMN	C4-C4A-N5	2.70	122.07	118.23
2	A	501	FMN	C4A-C10-N1	-2.66	118.56	124.73
2	F	501	FMN	C4A-C10-N1	-2.65	118.58	124.73
2	D	501	FMN	C4A-C10-N1	-2.64	118.59	124.73
2	B	501	FMN	C4A-C10-N1	-2.64	118.60	124.73
2	E	501	FMN	C4A-C10-N1	-2.64	118.60	124.73
2	C	501	FMN	C4A-C10-N1	-2.64	118.61	124.73
2	D	501	FMN	C10-N1-C2	2.25	121.40	116.90
2	F	501	FMN	C10-N1-C2	2.25	121.40	116.90
2	B	501	FMN	C10-N1-C2	2.24	121.37	116.90
2	C	501	FMN	C10-N1-C2	2.23	121.37	116.90
2	A	501	FMN	C10-N1-C2	2.23	121.36	116.90
2	C	501	FMN	O4-C4-C4A	-2.22	120.71	126.60
2	E	501	FMN	C10-N1-C2	2.22	121.34	116.90
2	E	501	FMN	O4-C4-C4A	-2.21	120.73	126.60
2	F	501	FMN	O4-C4-C4A	-2.20	120.76	126.60
2	D	501	FMN	O4-C4-C4A	-2.20	120.77	126.60
2	B	501	FMN	O4-C4-C4A	-2.19	120.79	126.60
2	A	501	FMN	O4-C4-C4A	-2.19	120.80	126.60
2	C	501	FMN	C4A-C4-N3	2.10	118.51	113.19
2	B	501	FMN	C4A-C4-N3	2.08	118.47	113.19
2	A	501	FMN	C4A-C10-N10	2.08	119.51	116.48
2	A	501	FMN	C4A-C4-N3	2.07	118.46	113.19
2	D	501	FMN	C4A-C4-N3	2.07	118.45	113.19
2	E	501	FMN	C4A-C4-N3	2.07	118.45	113.19
2	F	501	FMN	C4A-C4-N3	2.06	118.43	113.19
2	B	501	FMN	C4A-C10-N10	2.04	119.47	116.48
2	E	501	FMN	C4A-C10-N10	2.04	119.46	116.48
2	D	501	FMN	C4A-C10-N10	2.03	119.45	116.48
2	C	501	FMN	C4A-C10-N10	2.02	119.44	116.48
2	F	501	FMN	C4A-C10-N10	2.02	119.43	116.48

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	FMN	C1'-C2'-C3'-C4'
2	E	501	FMN	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
2	E	501	FMN	C5'-O5'-P-O2P
2	E	501	FMN	C5'-O5'-P-O3P
2	B	501	FMN	C4'-C5'-O5'-P
2	B	501	FMN	O2'-C2'-C3'-C4'
2	A	501	FMN	C4'-C5'-O5'-P
2	C	501	FMN	C4'-C5'-O5'-P
2	D	501	FMN	C4'-C5'-O5'-P
2	E	501	FMN	C2'-C3'-C4'-O4'
2	F	501	FMN	C2'-C3'-C4'-O4'
2	B	501	FMN	O2'-C2'-C3'-O3'
2	E	501	FMN	C4'-C5'-O5'-P
2	F	501	FMN	C4'-C5'-O5'-P
2	A	501	FMN	C5'-O5'-P-O2P
2	B	501	FMN	C5'-O5'-P-O3P
2	E	501	FMN	O3'-C3'-C4'-C5'
2	D	501	FMN	O2'-C2'-C3'-C4'
2	E	501	FMN	C2'-C3'-C4'-C5'
2	E	501	FMN	O3'-C3'-C4'-O4'
2	F	501	FMN	O3'-C3'-C4'-O4'
2	B	501	FMN	C2'-C3'-C4'-O4'
2	F	501	FMN	O3'-C3'-C4'-C5'
2	A	501	FMN	C2'-C3'-C4'-O4'
2	D	501	FMN	C2'-C3'-C4'-O4'
2	B	501	FMN	O4'-C4'-C5'-O5'
2	D	501	FMN	C2'-C1'-N10-C10

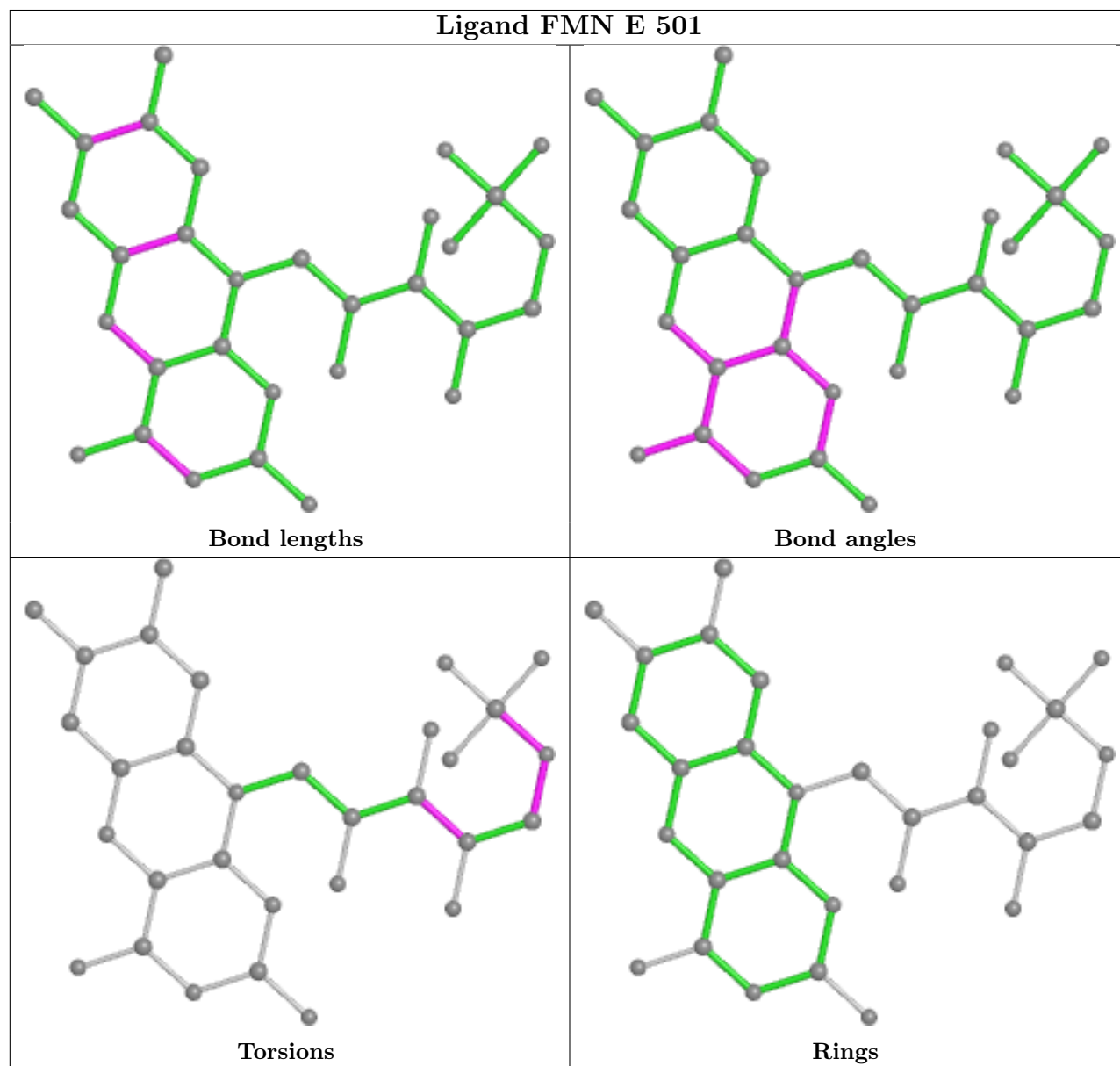
There are no ring outliers.

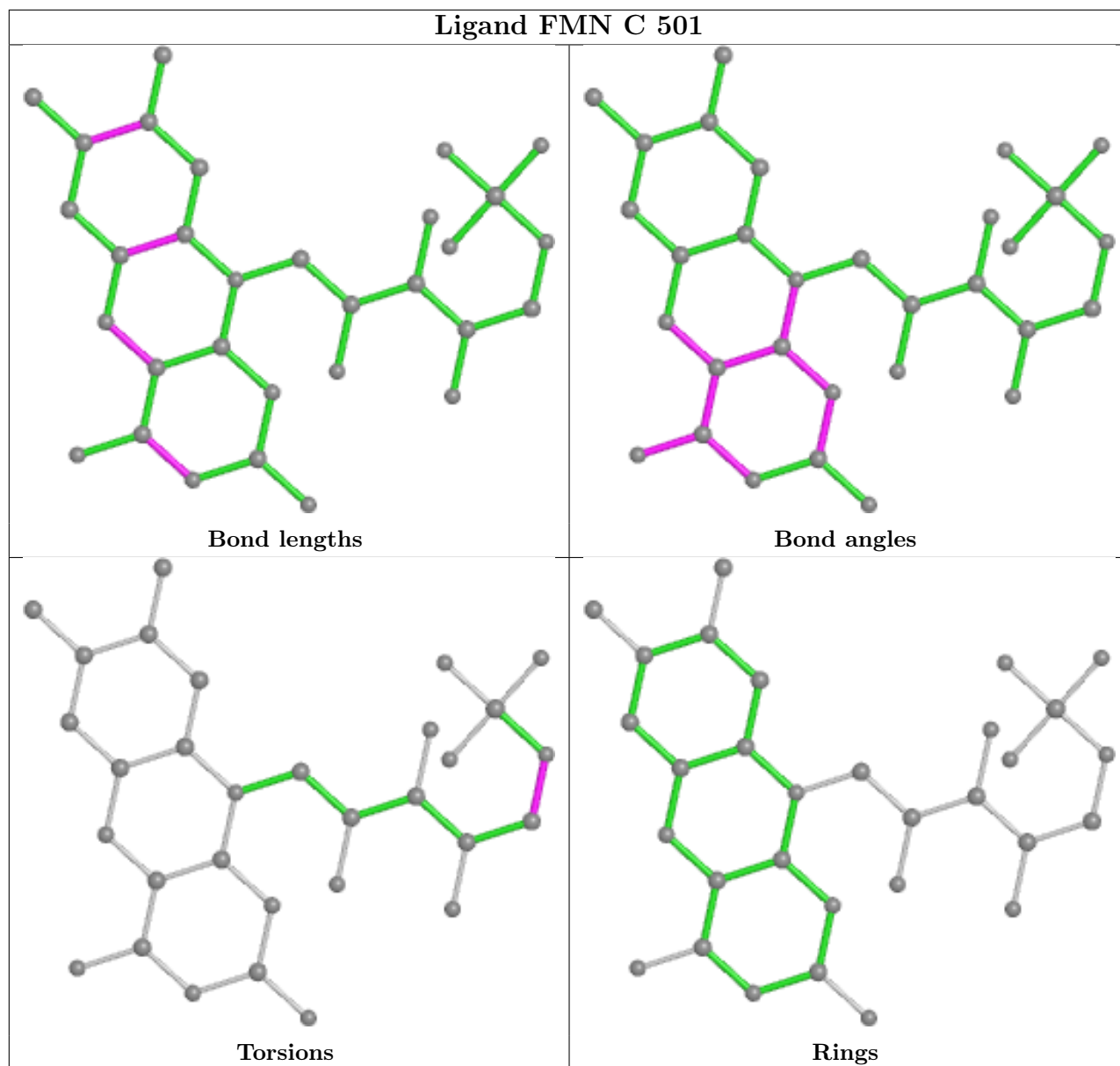
6 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	FMN	11	0
2	C	501	FMN	3	0
2	F	501	FMN	6	0
2	B	501	FMN	3	0
2	D	501	FMN	5	0
2	A	501	FMN	5	0

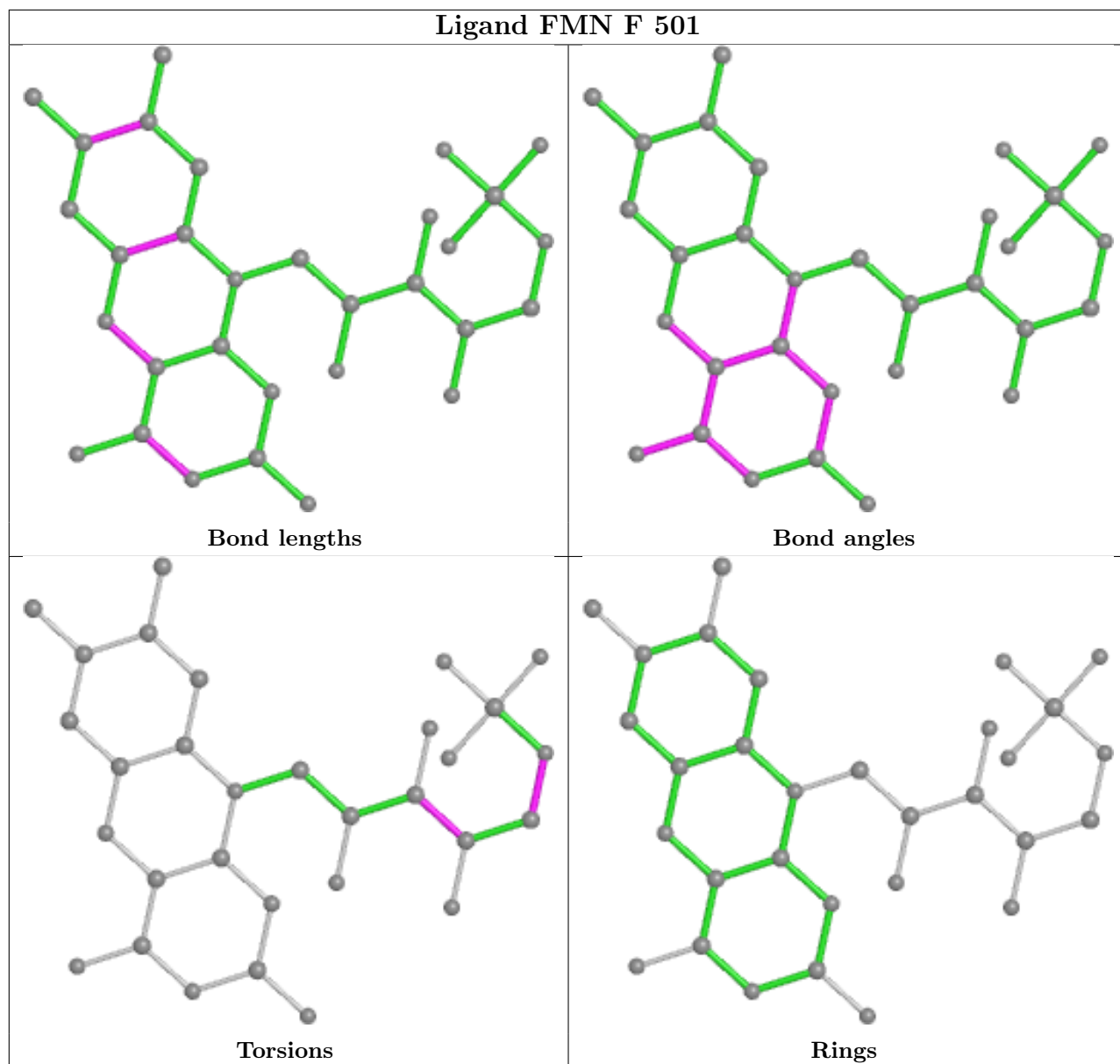
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

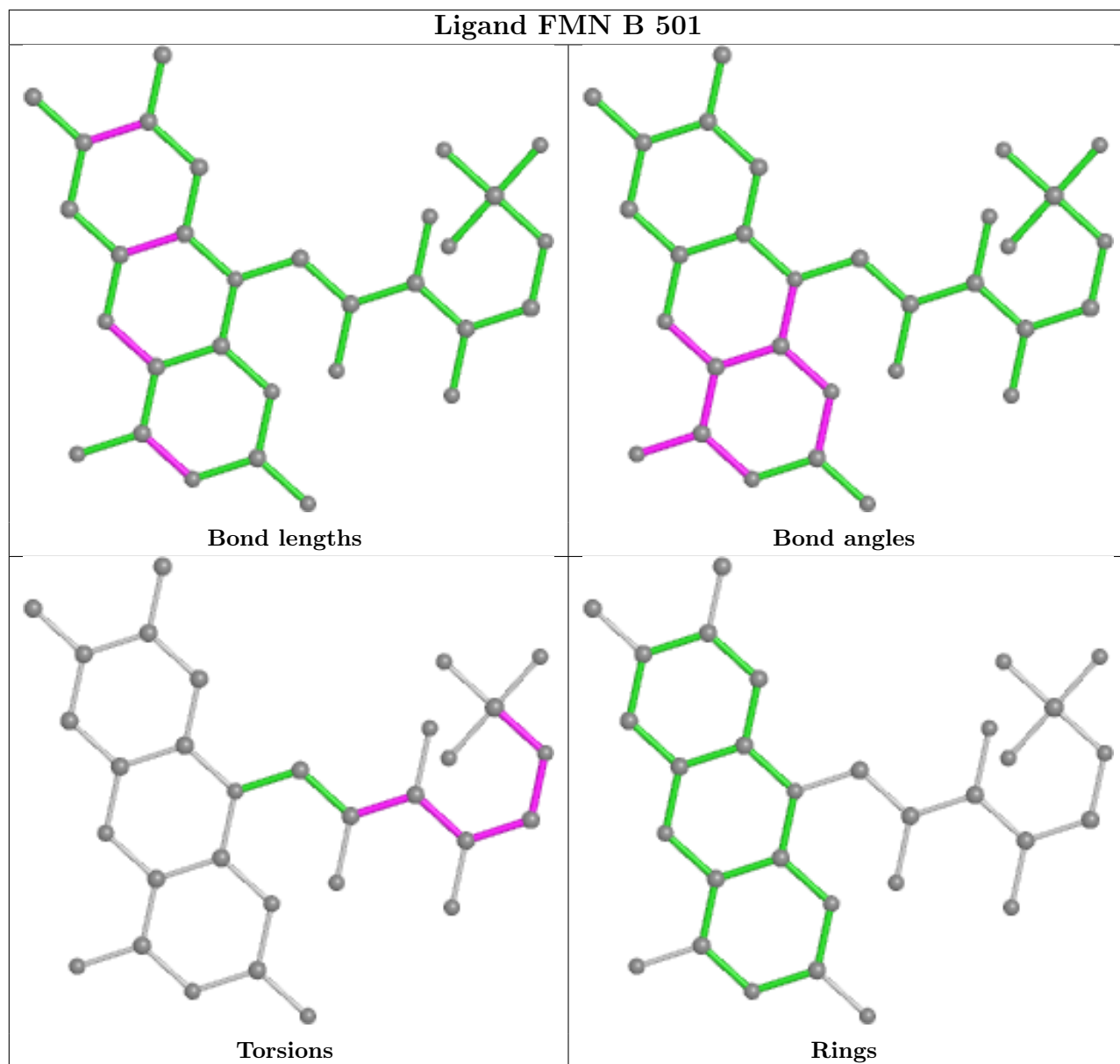
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

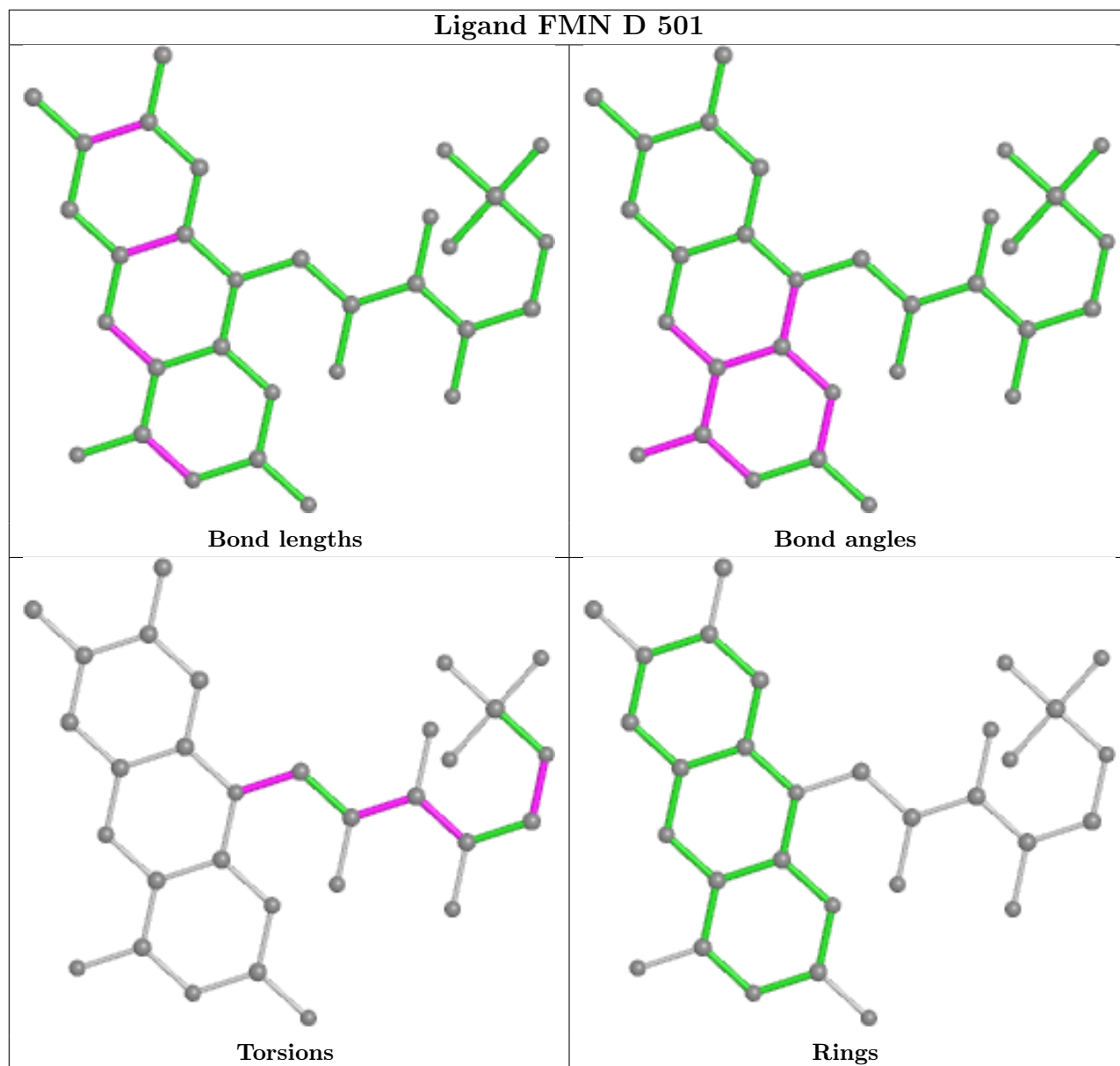


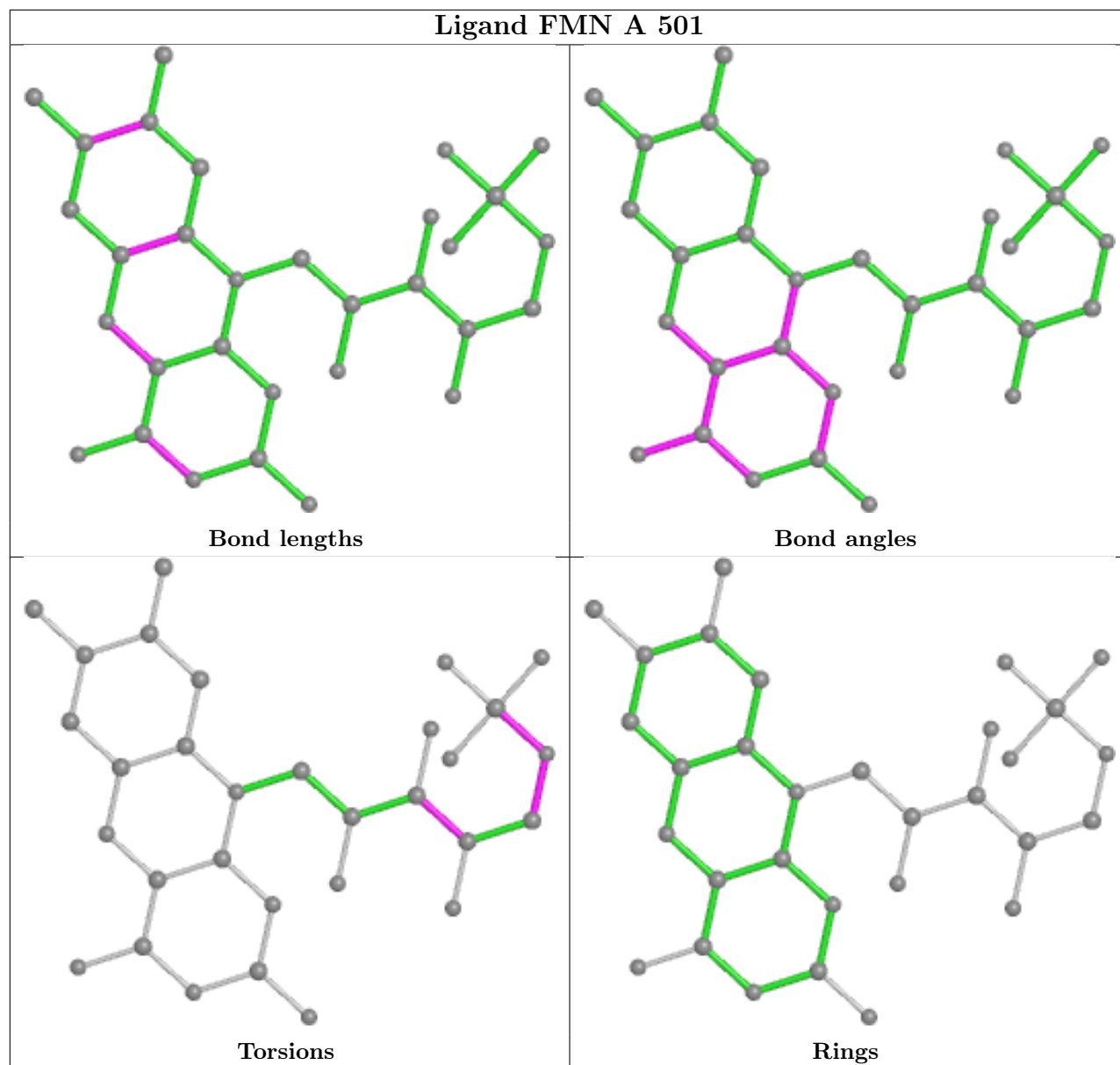












## 5.7 Other polymers [\(i\)](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	404/407 (99%)	-0.39	3 (0%) 87 91	27, 43, 68, 100	0
1	B	404/407 (99%)	-0.40	1 (0%) 95 97	25, 37, 58, 96	0
1	C	404/407 (99%)	-0.32	6 (1%) 73 81	36, 48, 67, 103	0
1	D	404/407 (99%)	0.14	22 (5%) 25 31	43, 64, 91, 111	0
1	E	404/407 (99%)	-0.11	11 (2%) 54 63	37, 56, 81, 109	0
1	F	404/407 (99%)	0.22	35 (8%) 10 12	44, 68, 95, 118	0
All	All	2424/2442 (99%)	-0.14	78 (3%) 47 56	25, 52, 86, 118	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	136	ALA	6.4
1	D	85	ILE	5.7
1	F	405	GLU	4.9
1	F	126	THR	4.8
1	D	79	GLU	4.7
1	E	389[A]	GLU	4.2
1	F	122	ALA	4.0
1	D	398	LYS	3.9
1	C	394[A]	GLU	3.8
1	F	389[A]	GLU	3.8
1	D	205[A]	GLN	3.6
1	F	394[A]	GLU	3.6
1	D	145	GLU	3.6
1	D	387	ASP	3.5
1	F	145	GLU	3.5
1	F	390	GLU	3.5
1	D	71	VAL	3.5
1	D	389[A]	GLU	3.4
1	E	325	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	136	ALA	3.3
1	F	265	TYR	3.3
1	D	391	VAL	3.2
1	F	150	VAL	3.2
1	F	142	ALA	3.2
1	F	123	VAL	3.0
1	B	405	GLU	3.0
1	D	91	ALA	3.0
1	E	387	ASP	3.0
1	F	398	LYS	3.0
1	D	388[A]	SER	2.9
1	E	365	LEU	2.9
1	D	405	GLU	2.9
1	F	400	VAL	2.9
1	F	44	THR	2.9
1	F	143	ALA	2.9
1	A	389[A]	GLU	2.9
1	D	404	ILE	2.8
1	F	180	ALA	2.8
1	A	398	LYS	2.7
1	F	89	LYS	2.7
1	E	394[A]	GLU	2.7
1	E	395	LEU	2.7
1	A	405	GLU	2.7
1	F	40	LEU	2.6
1	C	141	ASP	2.6
1	F	402	SER	2.6
1	E	405	GLU	2.5
1	F	146	ALA	2.5
1	D	187	LEU	2.5
1	D	394[A]	GLU	2.5
1	E	390	GLU	2.5
1	F	399	ARG	2.5
1	D	238	GLY	2.4
1	F	395	LEU	2.4
1	F	330	LYS	2.3
1	E	398	LYS	2.3
1	F	376	ASP	2.3
1	F	2	SER	2.3
1	E	150	VAL	2.3
1	F	147	ALA	2.3
1	F	392	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	154	VAL	2.2
1	F	266	LEU	2.2
1	E	329	PHE	2.1
1	F	152	ASN	2.1
1	F	267	VAL	2.1
1	F	93	ALA	2.1
1	C	356	VAL	2.1
1	F	92	LYS	2.1
1	C	391	VAL	2.1
1	F	386	MET	2.1
1	D	137	THR	2.1
1	D	207	THR	2.1
1	F	139	GLU	2.1
1	D	41	GLU	2.0
1	D	390	GLU	2.0
1	F	149	ALA	2.0
1	C	398	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

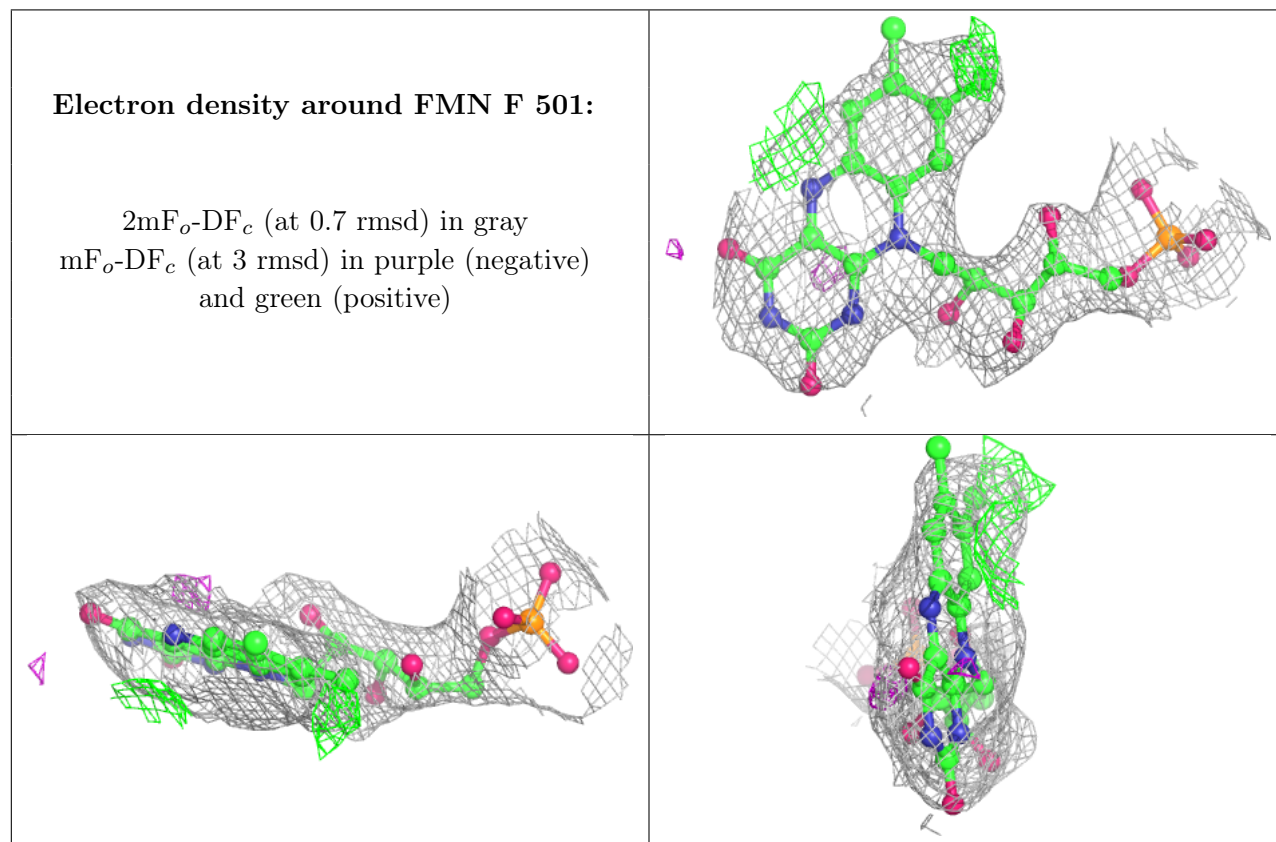
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

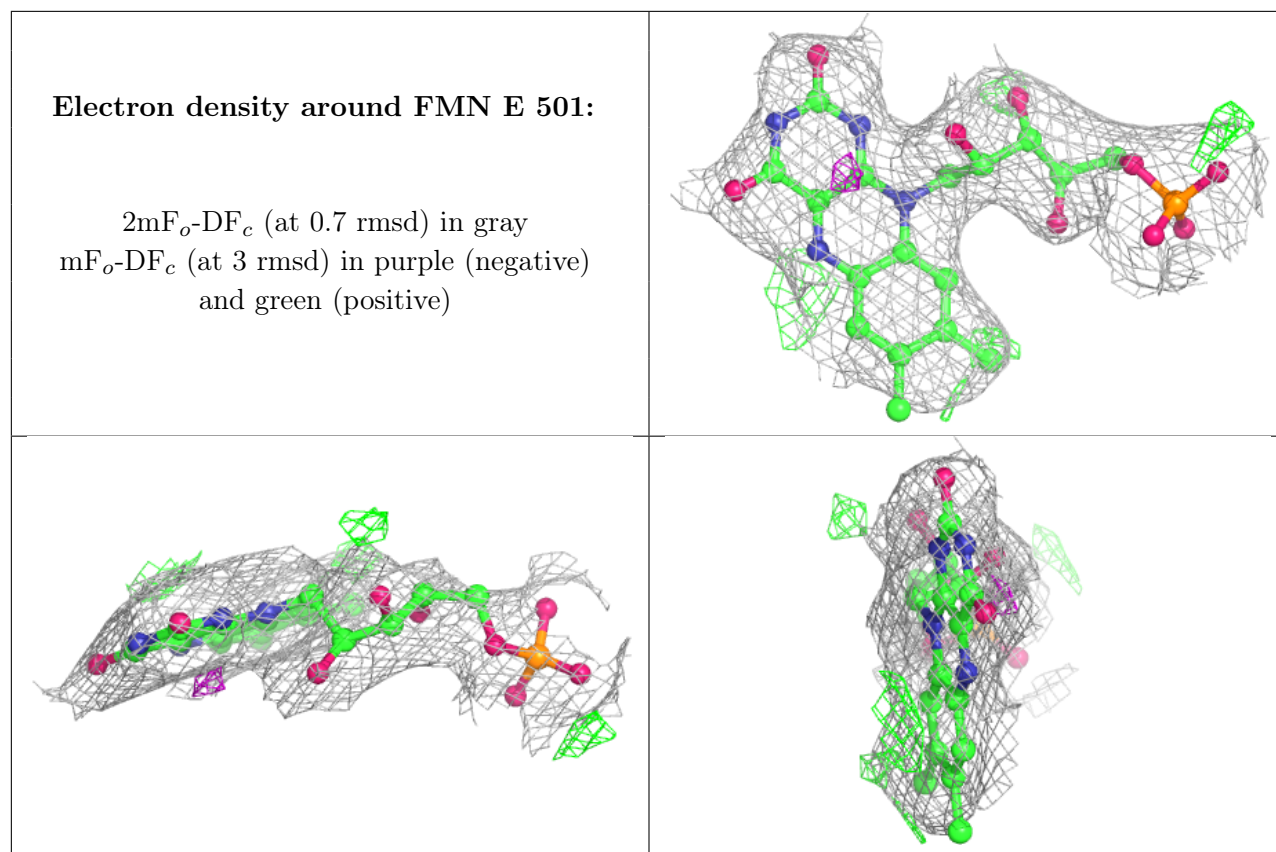
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FMN	F	501	31/31	0.91	0.19	47,63,81,89	0
2	FMN	E	501	31/31	0.92	0.19	46,60,72,79	0
2	FMN	D	501	31/31	0.92	0.19	47,63,77,92	0
2	FMN	A	501	31/31	0.94	0.19	30,43,60,75	0
2	FMN	B	501	31/31	0.95	0.21	28,41,58,66	0
2	FMN	C	501	31/31	0.96	0.16	37,49,62,68	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.

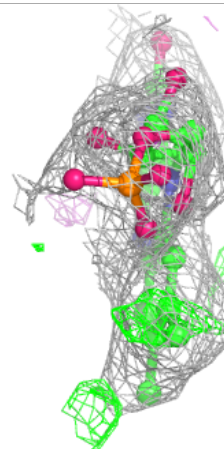
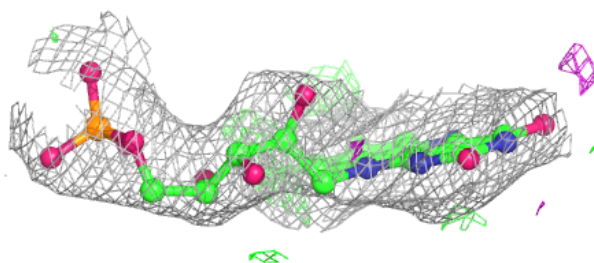
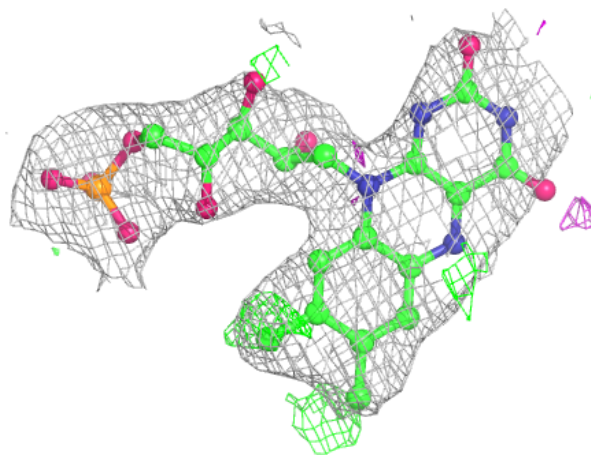






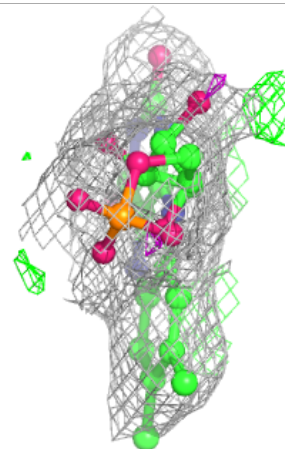
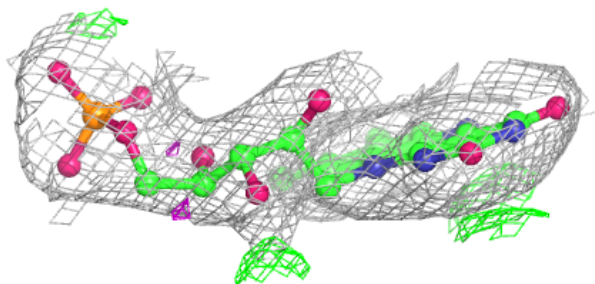
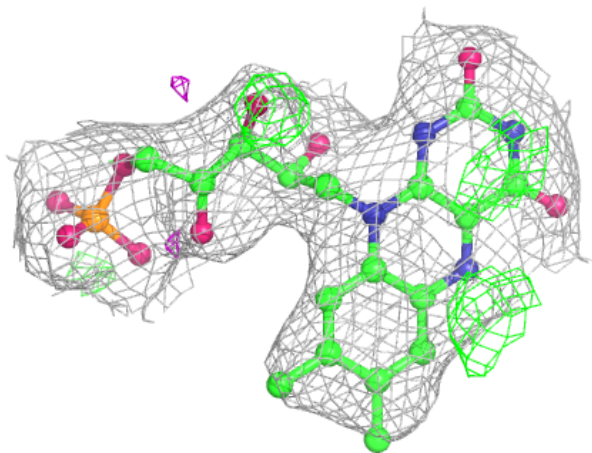
**Electron density around FMN D 501:**

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



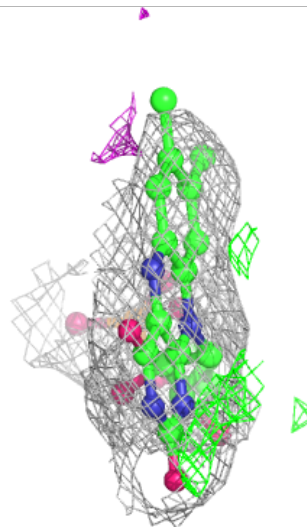
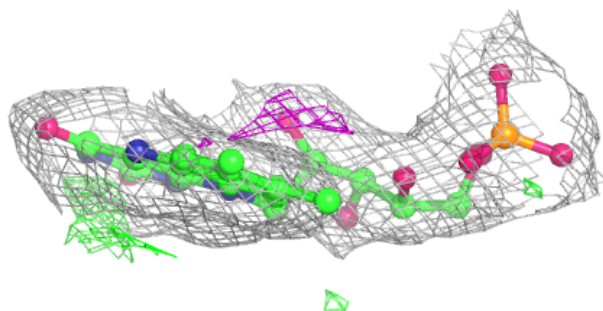
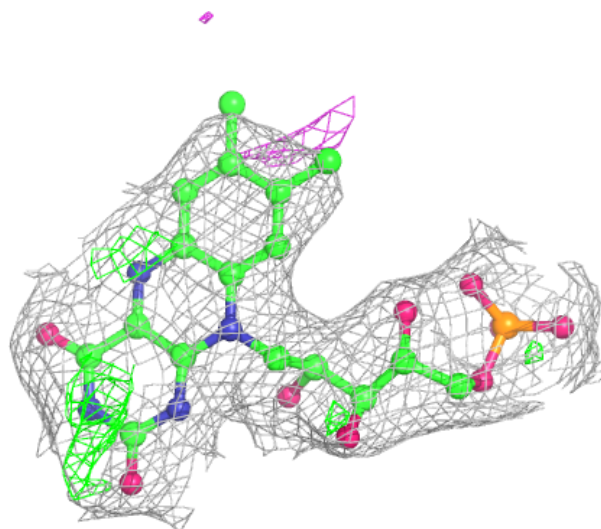
**Electron density around FMN A 501:**

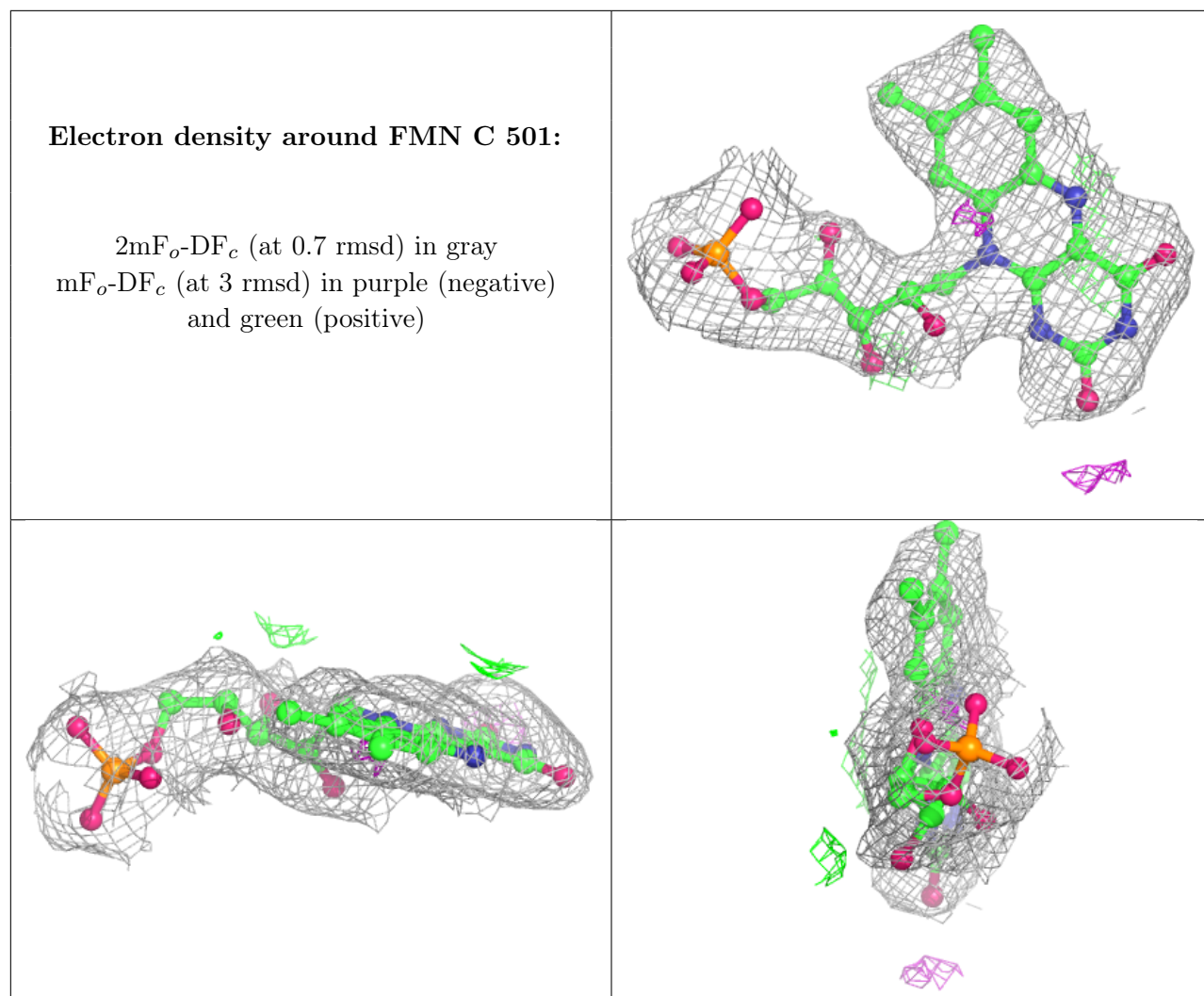
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around FMN 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.