



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:40 PM UTC

PDB ID : 7QFX / pdb_00007qfx
Title : Crystal structure of Old Yellow Enzyme AnOYE8 from *Aspergillus niger*
Authors : Robescu, M.S.; Loprete, G.; Vascon, F.; Gasparotto, M.; Filippini, F.;
Bergantino, E.; Cendron, L.
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

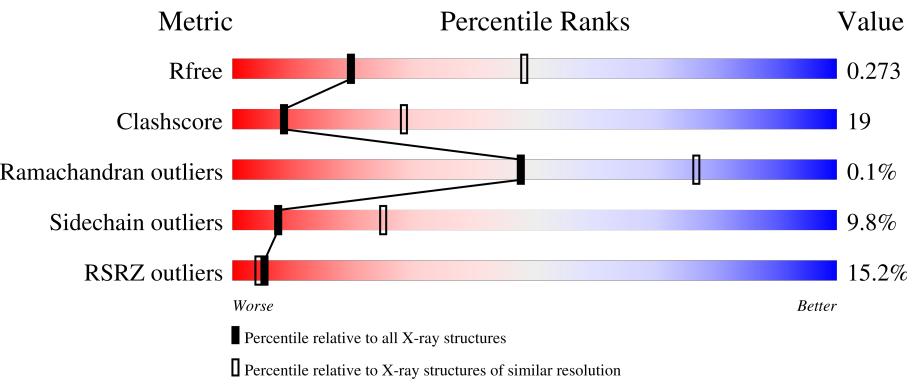
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 ≥ 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	7% 59% 32% 6%
1	C	422	9% 64% 30%
1	E	422	17% 57% 35%
1	G	422	26% 58% 33% 6%

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:

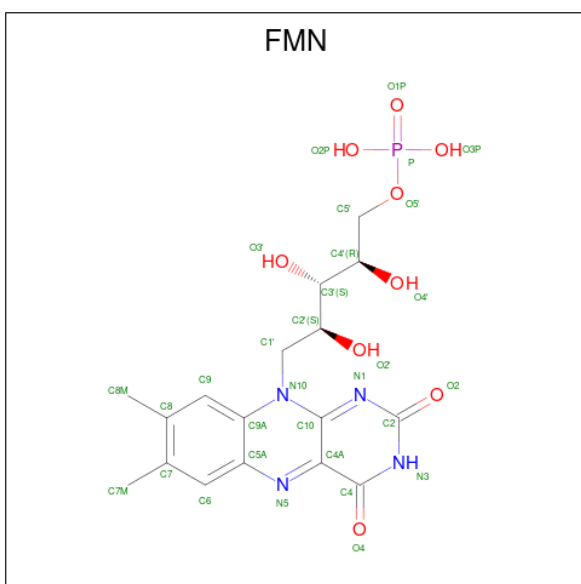
Chain	Residue	Modelled	Actual	Comment	Reference
B	422	PRO	-	expression tag	UNP A0A370CG11
C	427	PRO	-	expression tag	UNP A0A370CG11
E	422	PRO	-	expression tag	UNP A0A370CG11
G	422	PRO	-	expression tag	UNP A0A370CG11

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



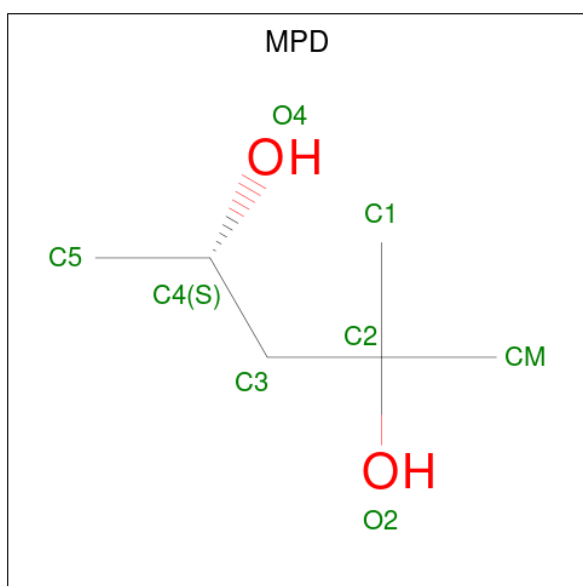
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P) (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 (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

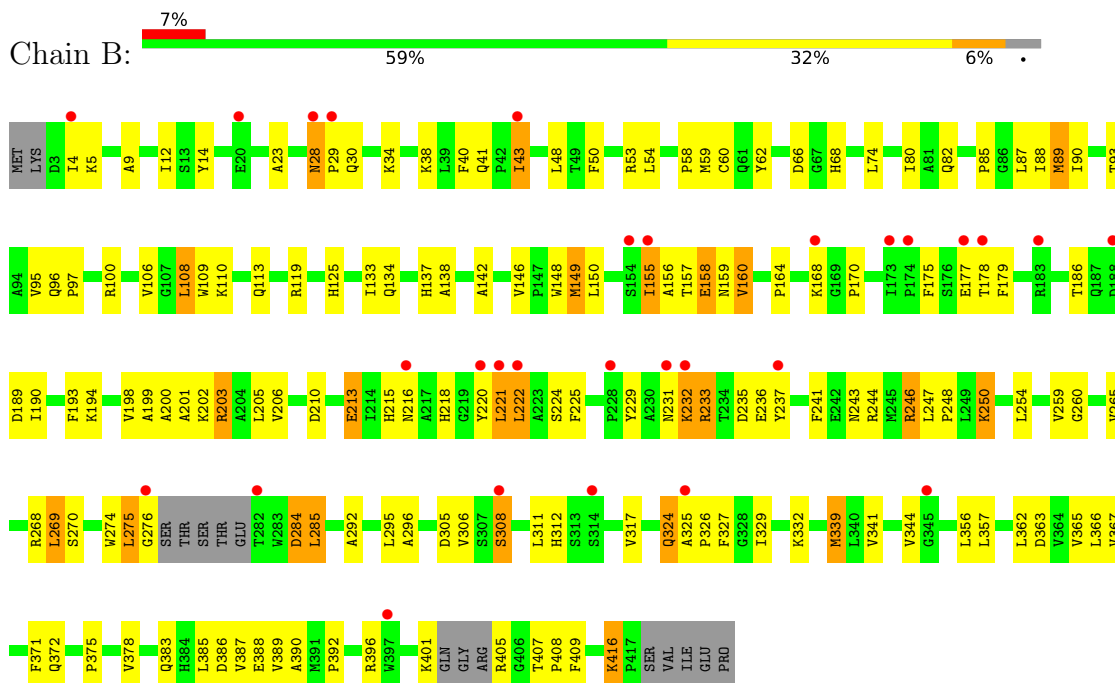
- Molecule 5 is water.

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		

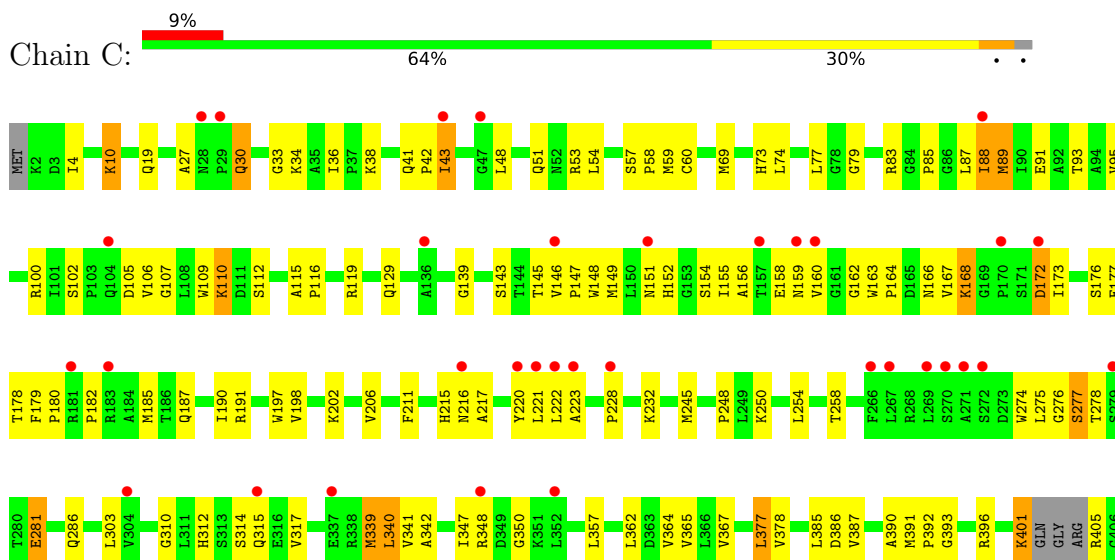
3 Residue-property plots [i](#)

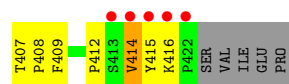
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: NADH-dependent flavin oxidoreductase

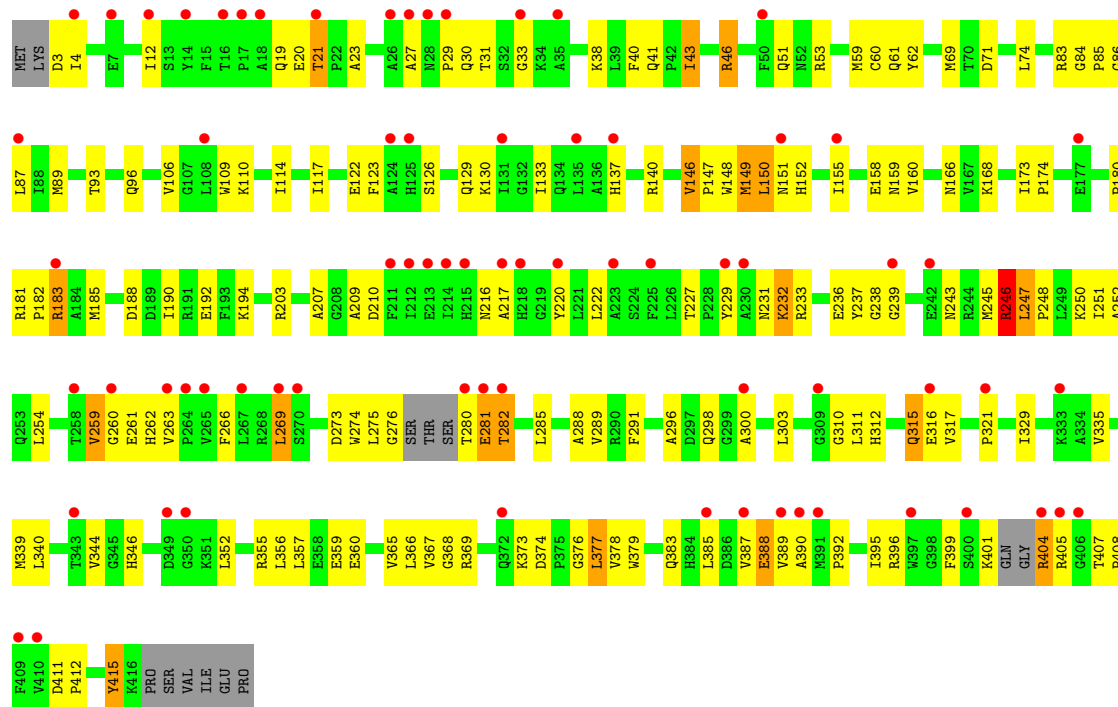


- Molecule 1: NADH-dependent flavin oxidoreductase

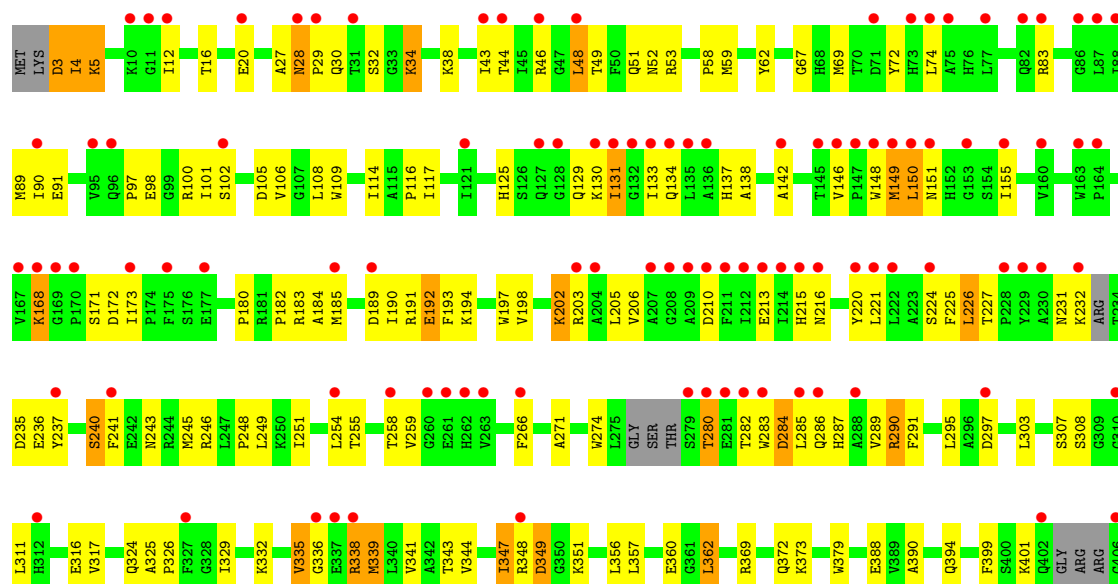


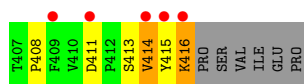


• Molecule 1: NADH-dependent flavin oxidoreductase



• Molecule 1: NADH-dependent flavin oxidoreductase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.241 , 0.266 (Not available) , 0.273	Depositor DCC
R_{free} test set	1942 reflections (4.43%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MPD, 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	0.84	0/3201	1.14	0/4345
1	C	0.68	0/3246	0.99	3/4407 (0.1%)
1	E	0.65	0/3220	0.99	4/4369 (0.1%)
1	G	0.68	1/3197 (0.0%)	0.99	4/4339 (0.1%)
All	All	0.72	1/12864 (0.0%)	1.03	11/17460 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	316	GLU	N-CA	-5.16	1.39	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	246	ARG	CA-C-O	-6.25	114.20	121.07
1	C	10	LYS	CA-CB-CG	-5.54	103.03	114.10
1	E	316	GLU	N-CA-C	-5.47	102.05	109.54
1	G	414	VAL	CA-C-N	-5.36	117.25	123.04
1	G	414	VAL	C-N-CA	-5.36	117.25	123.04
1	G	280	THR	CB-CA-C	-5.35	109.43	115.79
1	G	20	GLU	N-CA-C	-5.34	105.54	111.36
1	C	177	GLU	N-CA-C	-5.23	107.06	113.50
1	E	415	TYR	CA-C-N	-5.19	112.35	121.70
1	E	415	TYR	C-N-CA	-5.19	112.35	121.70
1	C	33	GLY	N-CA-C	-5.11	108.93	115.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3123	0	3089	118	0
1	C	3167	0	3133	107	0
1	E	3143	0	3108	135	0
1	G	3121	0	3078	136	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	4	0
3	C	31	0	19	4	0
3	E	31	0	19	4	0
3	G	31	0	19	4	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	478	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 19.

All (478) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:245:MET:HE2	1:G:249:LEU:HD11	1.65	0.78
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
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:C:69:MET:HE3	1:C:73:HIS:CB	2.25	0.66
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:296:ALA:HB2	1:E:339:MET:HE2	1.78	0.64
1:E:273:ASP:HB3	1:E:311:LEU:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:69:MET:HE3	1:C:73:HIS:HB3	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:G:69:MET:HE2	1:G:117:ILE:HG12	1.84	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:296:ALA:HB2	1:B:339:MET:HE2	1.85	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:B:110:LYS:HG2	1:B:113:GLN:CD	2.28	0.58
1:E:158:GLU:CD	1:E:158:GLU:H	2.11	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:176:SER:HG	1:C:179:PHE:HD1	1.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ASN:OD1	1:B:222:LEU:HB3	2.05	0.57
1:E:185:MET:HE2	1:E:190:ILE:HG12	1.86	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:B:225:PHE:O	1:B:244:ARG:HB3	2.07	0.55
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: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:B:158:GLU:CD	1:B:158:GLU:H	2.15	0.54
1:B:216:ASN:CG	1:B:222:LEU:HB3	2.32	0.54
1:B:275:LEU:O	1:B:276:GLY:C	2.50	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:E:259:VAL:HG13	1:E:263:VAL:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:148:TRP:NE1	1:C:149:MET:HE3	2.23	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
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:E:123:PHE:O	1:E:126:SER:OG	2.25	0.52
1:B:246:ARG:HG3	1:B:247:LEU:H	1.73	0.52
1:C:221:LEU:C	1:C:223:ALA:N	2.67	0.52
1:C:274:TRP:CG	1:C:317:VAL:HG22	2.44	0.52
1:C:221:LEU:C	1:C:223:ALA:H	2.17	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:58:PRO:HD3	1:B:89:MET:HE2	1.91	0.52
1:G:245:MET:CE	1:G:249:LEU:HD11	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:275:LEU:O	1:E:276:GLY:C	2.54	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
1:B:54:LEU:HD23	1:B:378:VAL:HG22	1.94	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:32:SER:C	1:G:34:LYS:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:MET:HE3	1:E:89:MET:HB2	1.65	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:286:GLN:CD	1:G:286:GLN:H	2.20	0.48
1:G:291:PHE:O	1:G:295:LEU:HG	2.13	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: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: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
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:G:59:MET:HE1	1:G:372:GLN:HG3	1.97	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: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:E:38:LYS:HA	1:E:41:GLN:CD	2.40	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:233:ARG:C	1:B:235:ASP:H	2.21	0.47
1:G:411:ASP:C	1:G:413:SER:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:172:ASP:C	1:G:182:PRO:HG2	2.40	0.47
1:C:158:GLU:HG3	1:C:164:PRO:HD2	1.96	0.46
1:E:151:ASN:O	1:E:152:HIS:C	2.58	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:247:LEU:HB3	1:E:248:PRO:HD3	1.97	0.46
1:E:298:GLN:HG2	1:E:300:ALA:H	1.80	0.46
1:G:245:MET:HE2	1:G:249:LEU:CD1	2.42	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
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:G:286:GLN:O	1:G:287:HIS:C	2.58	0.46
1:C:216:ASN:ND2	1:C:222:LEU:HB3	2.31	0.45
1:G:295:LEU:HB2	1:G:339:MET:HE1	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:233:ARG:C	1:E:238:GLY:HA3	2.41	0.45
1:G:98:GLU:H	1:G:98:GLU:CD	2.23	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: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:59:MET:HE3	1:E:59:MET:HB2	1.88	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
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:C:83:ARG:O	1:C:391:MET:HE1	2.17	0.44
1:E:69:MET:HE3	1:E:69:MET:HB3	1.81	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:148:TRP:CD1	1:C:149:MET:HE3	2.53	0.44
1:E:69:MET:HE2	1:E:117:ILE:HA	1.99	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
1:C:276:GLY:O	1:C:277:SER:C	2.60	0.44
1:C:367:VAL:HG11	1:C:377:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:ASN:CG	1:E:222:LEU:HB3	2.42	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: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
3:C:502:FMN:H2'	3:C:502:FMN:H9	2.00	0.43
1:G:27:ALA:O	1:G:28:ASN:C	2.61	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:C:286:GLN:H	1:C:286:GLN:CD	2.26	0.43
1:E:12:ILE:HG22	1:E:122:GLU:HG2	1.99	0.43
1:G:59:MET:C	1:G:91:GLU:HB3	2.43	0.43
1:G:339:MET:HE2	1:G:339:MET:HB2	1.85	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
1:C:339:MET:HB2	1:C:339:MET:HE2	1.75	0.43
1:G:411:ASP:C	1:G:413:SER:N	2.76	0.43
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:72:TYR:CD1	1:G:72:TYR:C	2.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:20:GLU:O	1:E:21:THR:C	2.62	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: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:G:335:VAL:O	1:G:336:GLY:C	2.62	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:C:185:MET:HE2	1:C:190:ILE:HG13	2.02	0.42
1:E:373:LYS:HE3	1:G:415:TYR:HB2	2.01	0.42
1:G:245:MET:O	1:G:246:ARG:C	2.63	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
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:C:414:VAL:O	1:C:415:TYR:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:31:THR:C	1:E:33:GLY:H	2.28	0.41
1:C:87:LEU:HD11	1:C:89:MET:HE2	2.01	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:C:148:TRP:HE1	1:C:149:MET:HE3	1.85	0.41
1:C:350:GLY:C	1:C:385:LEU:HD21	2.46	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: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:G:235:ASP:C	1:G:237:TYR:N	2.79	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:100:ARG:C	1:G:102:SER:H	2.28	0.40
1:B:66:ASP:HB3	1:B:68:HIS:CD2	2.52	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:E:374:ASP:C	1:E:376:GLY:H	2.30	0.40
1:G:134:GLN:CD	1:G:215:HIS:CD2	3.00	0.40
1:C:69:MET:O	1:C:116:PRO:HB3	2.21	0.40
1:C:245:MET:C	1:C:248:PRO:HD2	2.47	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

5.3.1 Protein backbone

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	100	100
1	C	409/422 (97%)	381 (93%)	27 (7%)	1 (0%)	43	72
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%)	48	77

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%)	287 (89%)	36 (11%)	6	20
1	C	329/337 (98%)	301 (92%)	28 (8%)	10	31
1	E	325/337 (96%)	295 (91%)	30 (9%)	8	27
1	G	324/337 (96%)	290 (90%)	34 (10%)	6	22
All	All	1301/1348 (96%)	1173 (90%)	128 (10%)	7	25

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	28	ASN
1	B	30	GLN
1	B	34	LYS
1	B	43	ILE
1	B	89	MET
1	B	108	LEU
1	B	149	MET
1	B	155	ILE
1	B	157	THR
1	B	158	GLU
1	B	159	ASN
1	B	160	VAL
1	B	168	LYS
1	B	203	ARG
1	B	213	GLU
1	B	221	LEU
1	B	222	LEU
1	B	232	LYS
1	B	233	ARG
1	B	246	ARG
1	B	250	LYS

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Mol	Chain	Res	Type
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	388	GLU
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	48	LEU
1	C	88	ILE
1	C	89	MET
1	C	110	LYS
1	C	155	ILE
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	191	ARG
1	C	250	LYS
1	C	277	SER
1	C	278	THR
1	C	281	GLU
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	414	VAL

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Mol	Chain	Res	Type
1	C	416	LYS
1	E	19	GLN
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	146	VAL
1	E	149	MET
1	E	150	LEU
1	E	159	ASN
1	E	183	ARG
1	E	232	LYS
1	E	246	ARG
1	E	247	LEU
1	E	251	ILE
1	E	259	VAL
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	378	VAL
1	E	388	GLU
1	E	404	ARG
1	E	405	ARG
1	E	407	THR
1	G	3	ASP
1	G	4	ILE
1	G	5	LYS
1	G	28	ASN
1	G	34	LYS
1	G	46	ARG
1	G	48	LEU
1	G	83	ARG
1	G	130	LYS
1	G	131	ILE
1	G	149	MET

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Mol	Chain	Res	Type
1	G	150	LEU
1	G	168	LYS
1	G	173	ILE
1	G	190	ILE
1	G	191	ARG
1	G	192	GLU
1	G	194	LYS
1	G	202	LYS
1	G	226	LEU
1	G	240	SER
1	G	280	THR
1	G	282	THR
1	G	284	ASP
1	G	290	ARG
1	G	297	ASP
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	96	GLN
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	324	GLN
1	C	30	GLN
1	C	76	HIS
1	C	129	GLN
1	C	187	GLN
1	C	216	ASN
1	C	253	GLN

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Mol	Chain	Res	Type
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	30	GLN
1	G	82	GLN
1	G	127	GLN
1	G	129	GLN
1	G	215	HIS
1	G	216	ASN
1	G	231	ASN
1	G	286	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	FMN	C	502	-	33,33,33	1.18	2 (6%)	48,50,50	2.14	17 (35%)
3	FMN	G	501	-	33,33,33	1.21	3 (9%)	48,50,50	1.81	11 (22%)
3	FMN	B	502	-	33,33,33	1.10	3 (9%)	48,50,50	1.44	7 (14%)
2	SO4	E	503	-	4,4,4	0.34	0	6,6,6	0.24	0
2	SO4	C	501	-	4,4,4	0.29	0	6,6,6	0.41	0
2	SO4	G	502	-	4,4,4	0.22	0	6,6,6	0.15	0
4	MPD	E	501	-	7,7,7	0.39	0	9,10,10	1.44	1 (11%)
3	FMN	E	502	-	33,33,33	1.21	3 (9%)	48,50,50	1.87	16 (33%)
2	SO4	B	501	-	4,4,4	0.27	0	6,6,6	0.24	0

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

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	FMN	C4A-N5	3.57	1.38	1.30
3	G	501	FMN	C4A-N5	3.45	1.38	1.30
3	B	502	FMN	C4A-N5	3.39	1.38	1.30
3	E	502	FMN	C4A-N5	3.05	1.37	1.30
3	G	501	FMN	C10-N1	2.84	1.39	1.33
3	E	502	FMN	C2'-C3'	-2.82	1.48	1.53
3	G	501	FMN	C1'-C2'	2.60	1.56	1.52
3	B	502	FMN	C10-N1	2.48	1.38	1.33
3	E	502	FMN	C10-N1	2.21	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	FMN	C4A-C10	-2.10	1.38	1.44
3	C	502	FMN	C4A-C10	-2.07	1.38	1.44

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	501	FMN	C4'-C3'-C2'	-5.94	103.68	113.57
3	C	502	FMN	O4'-C4'-C5'	-4.64	99.76	109.99
3	E	502	FMN	O4'-C4'-C5'	-4.20	100.73	109.99
3	C	502	FMN	C1'-C2'-C3'	4.13	120.85	109.66
3	C	502	FMN	C9A-C5A-N5	-3.98	118.23	122.45
3	E	502	FMN	O3'-C3'-C2'	-3.88	100.11	108.93
3	C	502	FMN	C5A-C9A-N10	3.86	121.46	117.97
3	G	501	FMN	O4'-C4'-C3'	-3.66	100.67	109.25
3	C	502	FMN	O2'-C2'-C3'	-3.60	100.82	109.25
3	C	502	FMN	C4'-C3'-C2'	-3.51	107.72	113.57
3	C	502	FMN	C4-N3-C2	-3.49	119.44	125.64
3	C	502	FMN	O4-C4-C4A	-3.49	117.33	126.53
3	B	502	FMN	O4-C4-C4A	-3.48	117.33	126.53
3	G	501	FMN	O3P-P-O5'	3.47	115.72	106.67
3	E	502	FMN	C4-N3-C2	-3.31	119.77	125.64
3	E	502	FMN	C4'-C3'-C2'	-3.31	108.07	113.57
3	G	501	FMN	C1'-C2'-C3'	3.25	118.48	109.66
3	G	501	FMN	C4-N3-C2	-3.25	119.86	125.64
3	C	502	FMN	C4A-C10-N10	3.12	120.95	116.48
4	E	501	MPD	O2-C2-C1	-3.02	98.58	107.99
3	C	502	FMN	O5'-P-O1P	3.01	114.58	106.44
3	E	502	FMN	C4A-C10-N10	3.00	120.77	116.48
3	B	502	FMN	C4-N3-C2	-2.91	120.47	125.64
3	B	502	FMN	C9A-C5A-N5	-2.90	119.37	122.45
3	C	502	FMN	C4A-C4-N3	2.87	120.55	113.25
3	G	501	FMN	C4A-C4-N3	2.81	120.41	113.25
3	E	502	FMN	O5'-C5'-C4'	-2.79	101.92	109.36
3	C	502	FMN	O3'-C3'-C2'	2.78	115.26	108.93
3	C	502	FMN	O3P-P-O5'	2.74	113.82	106.67
3	G	501	FMN	C4A-C10-N10	2.74	120.40	116.48
3	E	502	FMN	C10-C4A-N5	-2.69	119.31	124.81
3	E	502	FMN	O3'-C3'-C4'	2.63	114.92	108.93
3	B	502	FMN	O5'-C5'-C4'	-2.60	102.43	109.36
3	E	502	FMN	C4A-C4-N3	2.59	119.86	113.25
3	E	502	FMN	O4-C4-C4A	-2.58	119.72	126.53
3	G	501	FMN	C10-C4A-N5	-2.58	119.54	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	FMN	C4A-C4-N3	2.55	119.75	113.25
3	G	501	FMN	O4-C4-C4A	-2.54	119.84	126.53
3	B	502	FMN	O4'-C4'-C5'	-2.50	104.48	109.99
3	E	502	FMN	O4'-C4'-C3'	2.47	115.04	109.25
3	C	502	FMN	O2-C2-N1	-2.37	117.87	121.80
3	C	502	FMN	O2-C2-N3	2.34	123.08	118.58
3	E	502	FMN	C9A-C5A-N5	-2.33	119.98	122.45
3	C	502	FMN	O4'-C4'-C3'	2.29	114.61	109.25
3	E	502	FMN	O2-C2-N1	-2.29	118.00	121.80
3	E	502	FMN	O5'-P-O1P	-2.26	100.32	106.44
3	E	502	FMN	C4A-C10-N1	-2.24	119.11	124.59
3	E	502	FMN	O2P-P-O5'	2.16	112.31	106.67
3	G	501	FMN	O2-C2-N1	-2.15	118.22	121.80
3	G	501	FMN	C4A-C10-N1	-2.13	119.37	124.59
3	B	502	FMN	C4A-C10-N10	2.02	119.37	116.48
3	C	502	FMN	C9A-C9-C8	2.02	123.28	119.22

There are no chirality outliers.

All (37) 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'
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	N10-C1'-C2'-C3'
3	E	502	FMN	C1'-C2'-C3'-O3'
3	E	502	FMN	C1'-C2'-C3'-C4'

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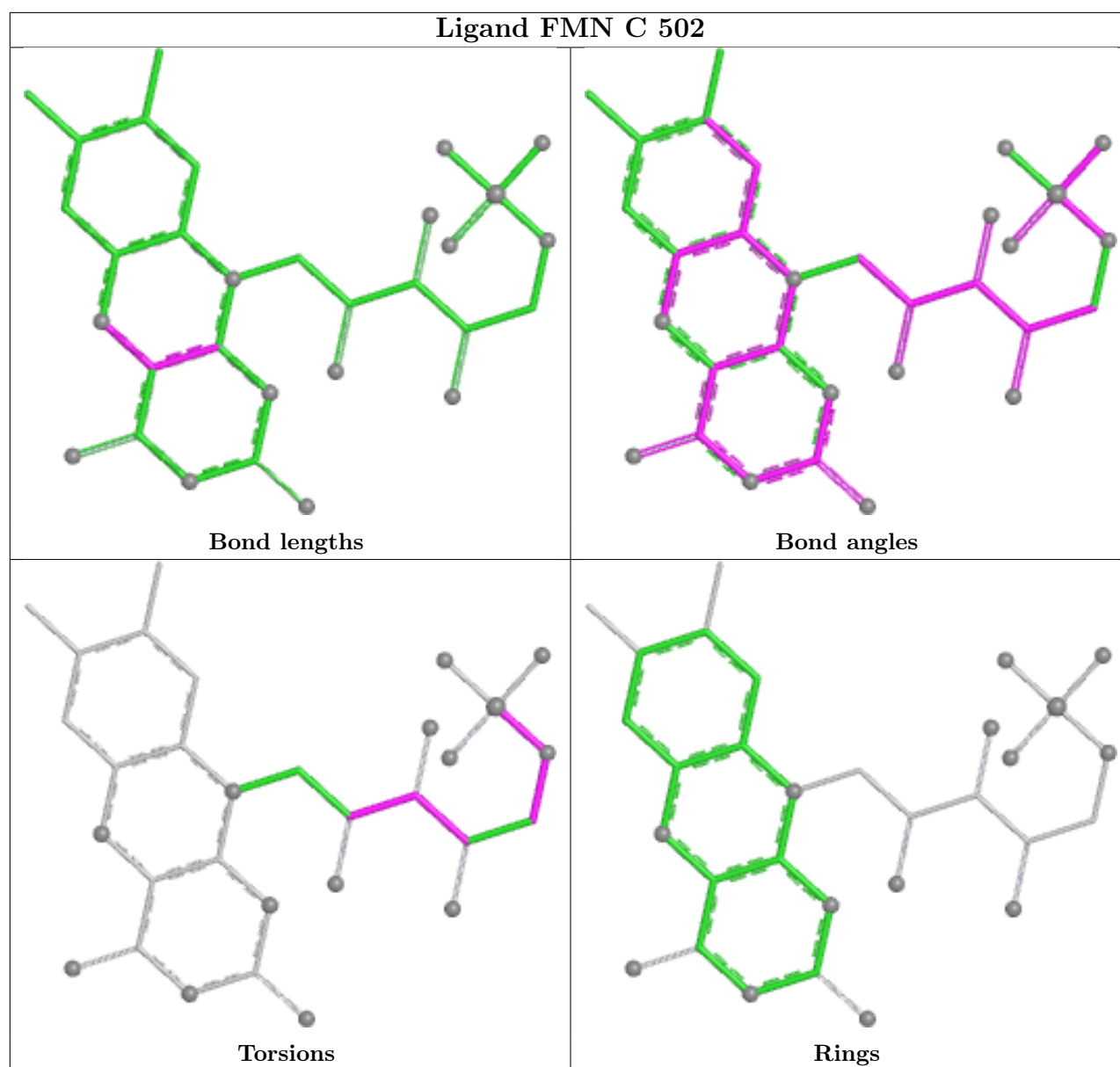
Mol	Chain	Res	Type	Atoms
3	E	502	FMN	O2'-C2'-C3'-O3'
3	E	502	FMN	O2'-C2'-C3'-C4'
3	E	502	FMN	C3'-C4'-C5'-O5'
3	E	502	FMN	O4'-C4'-C5'-O5'
3	E	502	FMN	C5'-O5'-P-O2P
3	E	502	FMN	C5'-O5'-P-O3P
3	C	502	FMN	O3'-C3'-C4'-C5'
3	B	502	FMN	O4'-C4'-C5'-O5'
3	G	501	FMN	O2'-C2'-C3'-O3'
3	G	501	FMN	O2'-C2'-C3'-C4'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

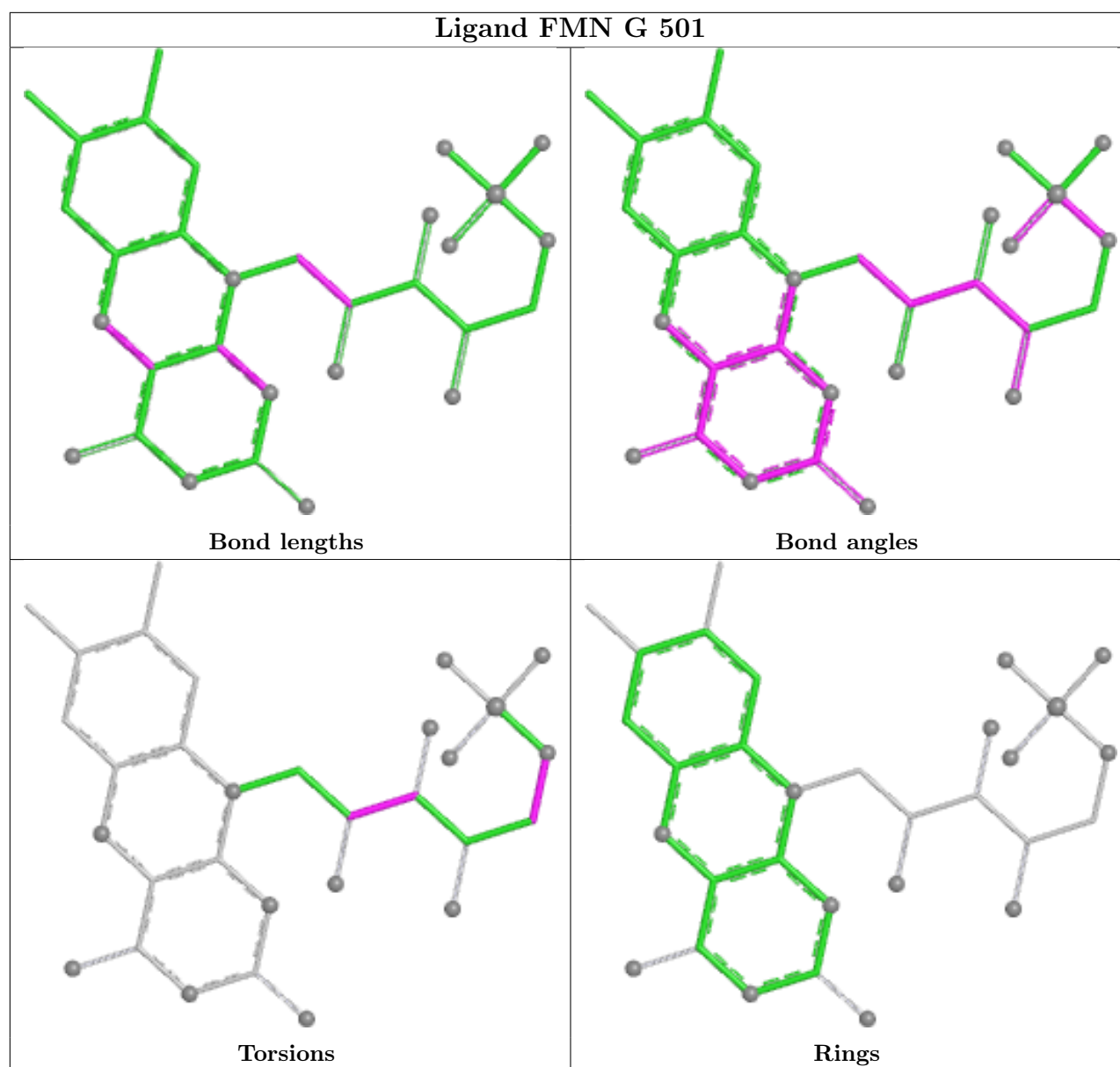
There are no ring outliers.

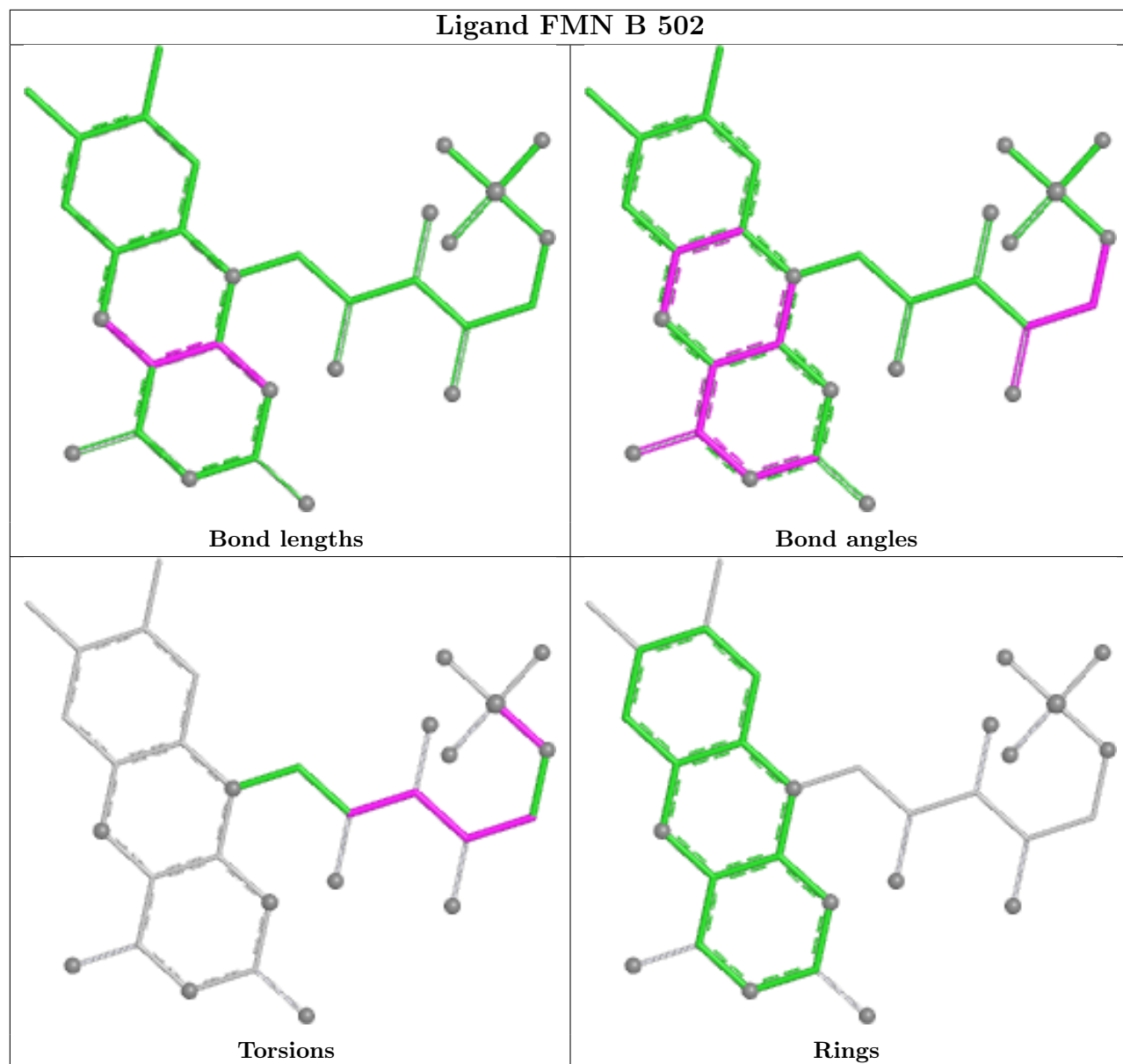
5 monomers are involved in 22 short contacts:

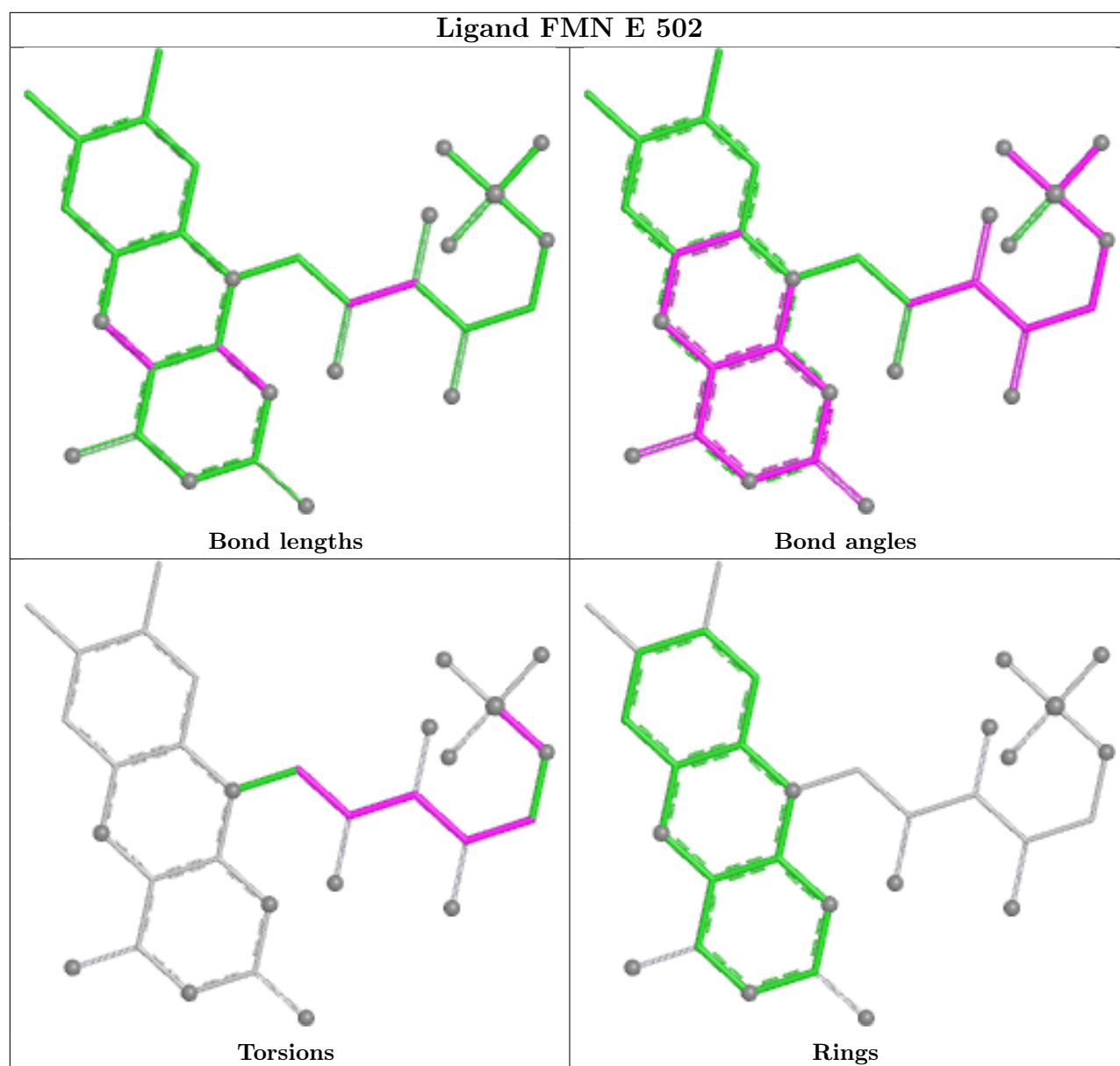
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	FMN	4	0
3	G	501	FMN	4	0
3	B	502	FMN	4	0
4	E	501	MPD	6	0
3	E	502	FMN	4	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	407/422 (96%)	0.91	29 (7%) 22 16	30, 69, 96, 114	0
1	C	413/422 (97%)	0.84	39 (9%) 14 10	38, 54, 80, 96	0
1	E	409/422 (96%)	1.23	72 (17%) 4 3	55, 74, 98, 120	0
1	G	407/422 (96%)	1.53	109 (26%) 1 1	30, 86, 127, 148	0
All	All	1636/1688 (96%)	1.13	249 (15%) 5 4	30, 71, 108, 148	0

All (249) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	349	ASP	5.8
1	C	414	VAL	5.6
1	G	229	TYR	5.4
1	G	208	GLY	5.2
1	G	150	LEU	5.0
1	C	415	TYR	4.7
1	G	210	ASP	4.7
1	E	264	PRO	4.7
1	E	269	LEU	4.6
1	C	413	SER	4.5
1	G	28	ASN	4.4
1	E	267	LEU	4.3
1	G	285	LEU	4.3
1	E	406	GLY	4.2
1	G	146	VAL	4.2
1	G	207	ALA	4.1
1	G	211	PHE	4.1
1	G	336	GLY	4.0
1	G	155	ILE	4.0
1	G	212	ILE	4.0
1	C	28	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	G	402	GLN	3.9
1	B	221	LEU	3.8
1	G	87	LEU	3.8
1	G	128	GLY	3.8
1	B	28	ASN	3.8
1	E	405	ARG	3.7
1	G	133	ILE	3.7
1	G	160	VAL	3.7
1	G	75	ALA	3.6
1	G	209	ALA	3.6
1	C	29	PRO	3.6
1	G	279	SER	3.6
1	E	281	GLU	3.6
1	B	231	ASN	3.6
1	G	74	LEU	3.6
1	G	86	GLY	3.5
1	E	151	ASN	3.5
1	B	29	PRO	3.5
1	E	214	ILE	3.5
1	E	239	GLY	3.5
1	G	280	THR	3.5
1	C	47	GLY	3.4
1	C	220	TYR	3.4
1	B	43	ILE	3.3
1	C	159	ASN	3.3
1	G	168	LYS	3.3
1	B	345	GLY	3.3
1	E	258	THR	3.3
1	E	28	ASN	3.2
1	G	241	PHE	3.2
1	C	269	LEU	3.2
1	E	218	HIS	3.2
1	C	160	VAL	3.2
1	G	262	HIS	3.1
1	E	280	THR	3.1
1	B	173	ILE	3.1
1	G	29	PRO	3.1
1	B	168	LYS	3.0
1	G	48	LEU	3.0
1	G	228	PRO	3.0
1	E	225	PHE	3.0
1	C	183	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	12	ILE	3.0
1	E	108	LEU	3.0
1	C	422	PRO	3.0
1	B	228	PRO	2.9
1	G	224	SER	2.9
1	G	263	VAL	2.9
1	G	170	PRO	2.9
1	C	272	SER	2.9
1	G	136	ALA	2.9
1	B	4	ILE	2.9
1	G	163	TRP	2.9
1	E	183	ARG	2.9
1	B	237	TYR	2.8
1	B	232	LYS	2.8
1	C	172	ASP	2.8
1	C	221	LEU	2.8
1	E	410	VAL	2.8
1	C	271	ALA	2.8
1	G	220	TYR	2.8
1	G	221	LEU	2.8
1	G	260	GLY	2.8
1	E	389	VAL	2.7
1	C	43	ILE	2.7
1	G	31	THR	2.7
1	E	265	VAL	2.7
1	G	148	TRP	2.7
1	G	185	MET	2.7
1	G	153	GLY	2.7
1	B	20	GLU	2.7
1	E	270	SER	2.7
1	G	135	LEU	2.7
1	G	147	PRO	2.7
1	G	214	ILE	2.6
1	E	14	TYR	2.6
1	G	46	ARG	2.6
1	E	21	THR	2.6
1	C	216	ASN	2.6
1	E	212	ILE	2.6
1	C	270	SER	2.6
1	E	27	ALA	2.6
1	G	288	ALA	2.6
1	G	215	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	343	THR	2.6
1	G	131	ILE	2.6
1	E	124	ALA	2.6
1	E	263	VAL	2.6
1	B	154	SER	2.6
1	G	130	LYS	2.6
1	C	222	LEU	2.6
1	C	157	THR	2.6
1	E	35	ALA	2.6
1	G	83	ARG	2.5
1	B	276	GLY	2.5
1	E	220	TYR	2.5
1	G	95	VAL	2.5
1	G	337	GLU	2.5
1	B	222	LEU	2.5
1	G	132	GLY	2.5
1	E	213	GLU	2.5
1	C	279	SER	2.5
1	E	17	PRO	2.5
1	E	155	ILE	2.5
1	G	43	ILE	2.5
1	G	90	ILE	2.5
1	G	283	TRP	2.5
1	G	222	LEU	2.5
1	G	11	GLY	2.5
1	G	96	GLN	2.5
1	G	145	THR	2.5
1	B	308	SER	2.4
1	B	314	SER	2.4
1	G	338	ARG	2.4
1	C	136	ALA	2.4
1	B	183	ARG	2.4
1	E	404	ARG	2.4
1	E	177	GLU	2.4
1	E	300	ALA	2.4
1	B	178	THR	2.4
1	B	282	THR	2.4
1	E	125	HIS	2.4
1	C	267	LEU	2.4
1	E	33	GLY	2.4
1	E	217	ALA	2.4
1	G	415	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	258	THR	2.4
1	G	216	ASN	2.4
1	E	211	PHE	2.4
1	G	254	LEU	2.4
1	B	155	ILE	2.4
1	E	131	ILE	2.4
1	C	181	ARG	2.3
1	G	348	ARG	2.3
1	C	337	GLU	2.3
1	E	223	ALA	2.3
1	E	230	ALA	2.3
1	E	316	GLU	2.3
1	G	44	THR	2.3
1	G	237	TYR	2.3
1	E	309	GLY	2.3
1	C	266	PHE	2.3
1	G	409	PHE	2.3
1	B	325	ALA	2.3
1	G	127	GLN	2.3
1	E	215	HIS	2.3
1	G	88	ILE	2.3
1	G	282	THR	2.3
1	C	348	ARG	2.3
1	G	261	GLU	2.3
1	G	82	GLN	2.3
1	E	397	TRP	2.3
1	G	121	ILE	2.3
1	E	229	TYR	2.3
1	E	50	PHE	2.3
1	G	175	PHE	2.3
1	E	18	ALA	2.3
1	G	213	GLU	2.3
1	G	312	HIS	2.3
1	C	304	VAL	2.3
1	E	350	GLY	2.3
1	G	310	GLY	2.3
1	B	216	ASN	2.2
1	E	7	GLU	2.2
1	G	416	LYS	2.2
1	C	88	ILE	2.2
1	G	173	ILE	2.2
1	B	397	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	167	VAL	2.2
1	G	406	GLY	2.2
1	G	327	PHE	2.2
1	G	142	ALA	2.2
1	B	174	PRO	2.2
1	E	387	VAL	2.2
1	G	169	GLY	2.2
1	E	242	GLU	2.2
1	G	134	GLN	2.2
1	G	71	ASP	2.2
1	E	333	LYS	2.2
1	C	352	LEU	2.2
1	G	77	LEU	2.2
1	G	164	PRO	2.2
1	E	16	THR	2.2
1	E	409	PHE	2.2
1	G	177	GLU	2.2
1	C	104	GLN	2.1
1	E	321	PRO	2.1
1	G	297	ASP	2.1
1	C	416	LYS	2.1
1	E	87	LEU	2.1
1	E	385	LEU	2.1
1	G	102	SER	2.1
1	E	4	ILE	2.1
1	E	372	GLN	2.1
1	G	286	GLN	2.1
1	C	146	VAL	2.1
1	G	414	VAL	2.1
1	G	232	LYS	2.1
1	G	411	ASP	2.1
1	E	135	LEU	2.1
1	B	220	TYR	2.1
1	C	223	ALA	2.1
1	B	177	GLU	2.1
1	G	20	GLU	2.1
1	C	315	GLN	2.1
1	C	170	PRO	2.1
1	C	228	PRO	2.1
1	G	151	ASN	2.1
1	B	188	ASP	2.1
1	G	189	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	266	PHE	2.1
1	G	281	GLU	2.1
1	E	391	MET	2.1
1	G	73	HIS	2.1
1	E	29	PRO	2.1
1	E	137	HIS	2.0
1	C	151	ASN	2.0
1	G	203	ARG	2.0
1	E	26	ALA	2.0
1	E	390	ALA	2.0
1	G	149	MET	2.0
1	E	400	SER	2.0
1	E	260	GLY	2.0
1	G	12	ILE	2.0
1	E	282	THR	2.0
1	G	204	ALA	2.0
1	G	230	ALA	2.0
1	G	10	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MPD	E	501	8/8	0.59	0.22	75,78,80,81	0
2	SO4	E	503	5/5	0.76	0.23	33,33,33,33	5
2	SO4	G	502	5/5	0.87	0.24	33,33,33,33	5
2	SO4	C	501	5/5	0.88	0.28	48,49,49,51	5
3	FMN	E	502	31/31	0.89	0.16	33,33,33,33	0

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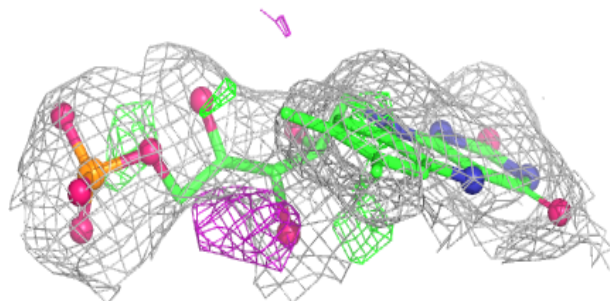
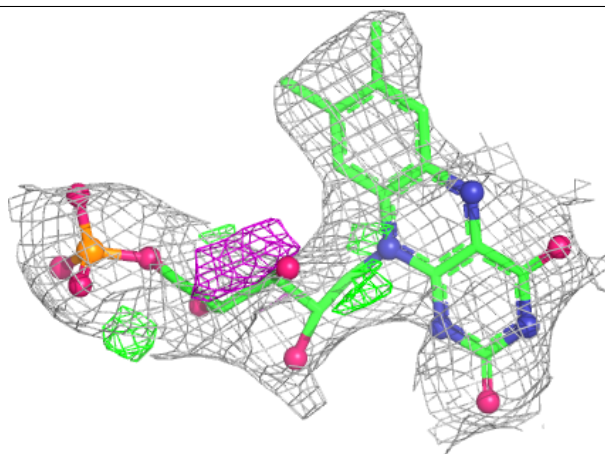
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FMN	G	501	31/31	0.89	0.11	33,33,33,33	0
3	FMN	B	502	31/31	0.89	0.16	33,33,33,33	0
3	FMN	C	502	31/31	0.91	0.19	33,33,33,33	0
2	SO4	B	501	5/5	0.93	0.20	55,55,56,58	5

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.

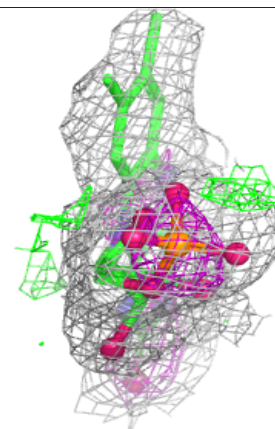
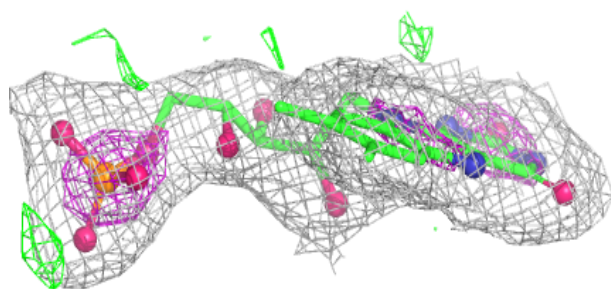
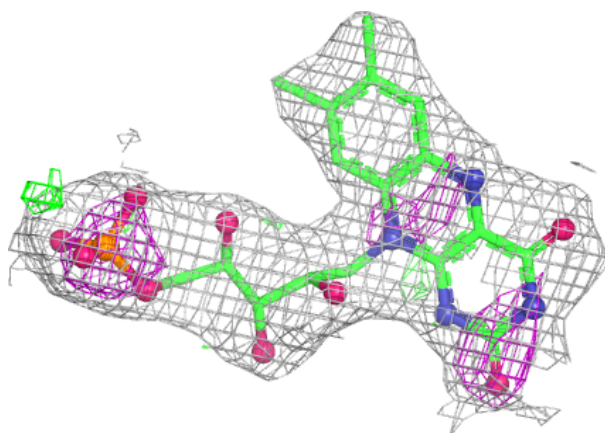
Electron density around FMN E 502:

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



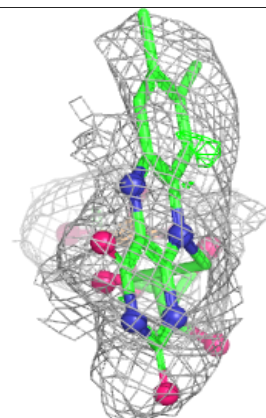
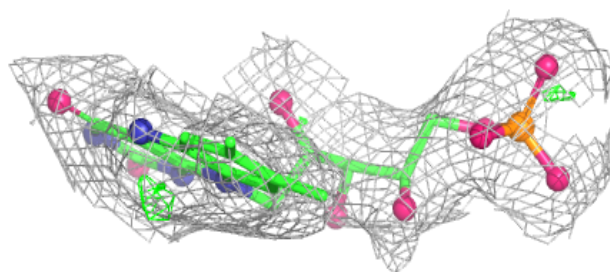
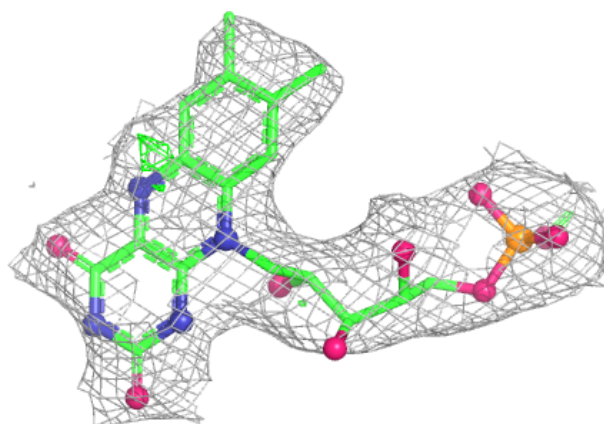
Electron density around FMN G 501:

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



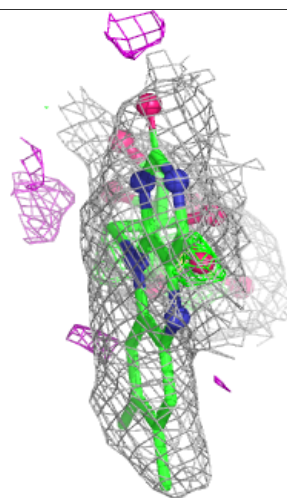
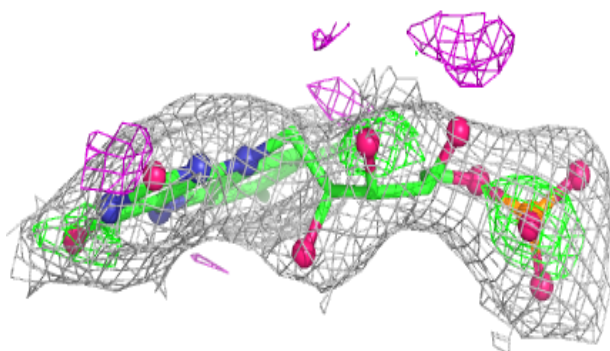
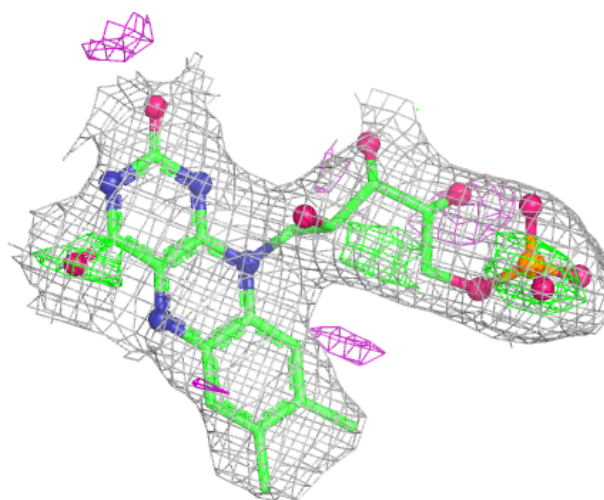
Electron density around FMN B 502:

$2mF_o - DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.