



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:50 AM EDT

PDB ID : 2OHI / pdb_00002ohi
Title : Crystal Structure of coenzyme F420H2 oxidase (FprA), a diiron flavoprotein, reduced state
Authors : Seedorf, H.; Warkentin, E.; Ermler, U.
Deposited on : 2007-01-10
Resolution : 2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

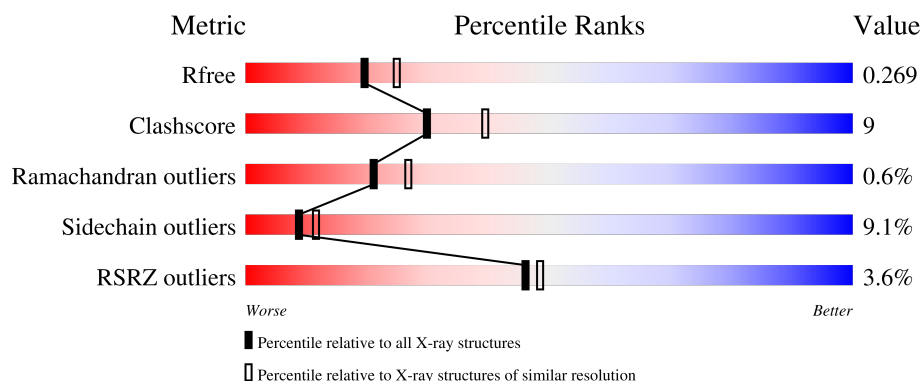
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

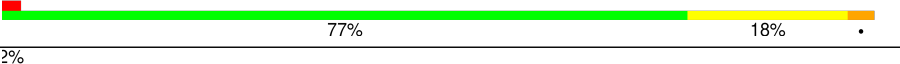
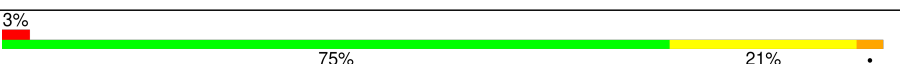
The reported resolution of this entry is 2.30 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	404	
1	B	404	
1	D	404	
1	E	404	
1	G	404	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	404	7% 75% 22%
1	I	404	4% 75% 21%
1	J	404	3% 78% 18%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 25966 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 Type A flavoprotein fprA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	1	0
			3166	2014	526	604	22			
1	B	403	Total	C	N	O	S	0	0	0
			3162	2012	525	603	22			
1	D	403	Total	C	N	O	S	0	3	0
			3178	2022	530	604	22			
1	E	403	Total	C	N	O	S	0	1	0
			3168	2016	527	603	22			
1	G	403	Total	C	N	O	S	0	1	0
			3166	2014	526	604	22			
1	H	403	Total	C	N	O	S	0	0	0
			3162	2012	525	603	22			
1	I	403	Total	C	N	O	S	0	0	0
			3162	2012	525	603	22			
1	J	403	Total	C	N	O	S	0	2	0
			3169	2016	527	604	22			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

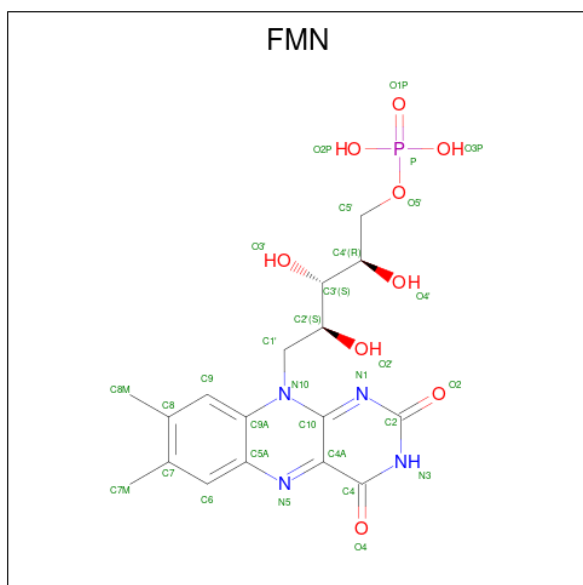
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		
2	B	2	Total	Fe	0	0
			2	2		
2	D	2	Total	Fe	0	0
			2	2		
2	E	2	Total	Fe	0	0
			2	2		
2	G	2	Total	Fe	0	0
			2	2		
2	H	2	Total	Fe	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	2	Total	Fe	0	0
			2	2		
2	J	2	Total	Fe	0	0
			2	2		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



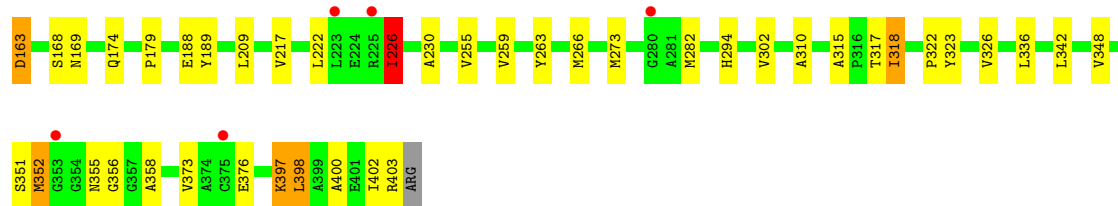
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	I	1	Total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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

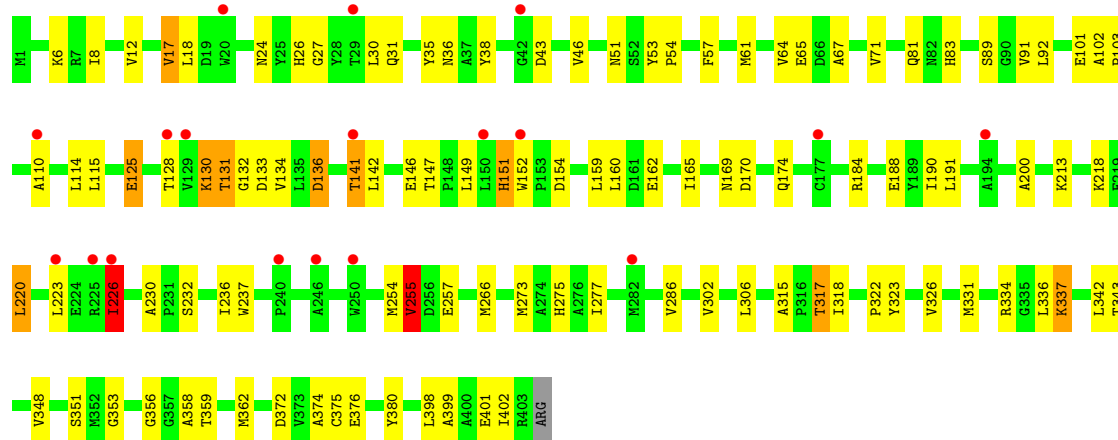
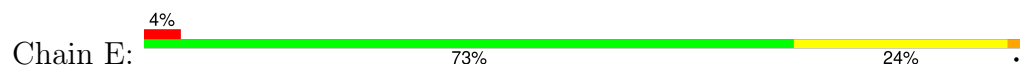
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total 1	Cl 1	0	0
4	H	1	Total 1	Cl 1	0	0
4	J	2	Total 2	Cl 2	0	0

- Molecule 5 is water.

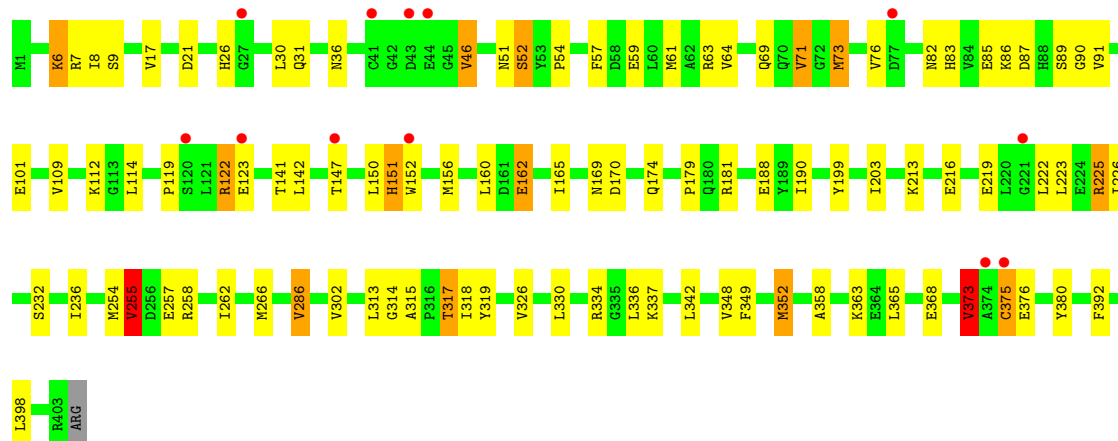
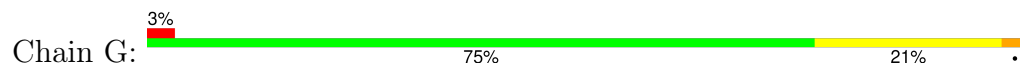
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	46	Total 46	O 46	0	0
5	B	47	Total 47	O 47	0	0
5	D	57	Total 57	O 57	0	0
5	E	42	Total 42	O 42	0	0
5	G	50	Total 50	O 50	0	0
5	H	45	Total 45	O 45	0	0
5	I	33	Total 33	O 33	0	0
5	J	45	Total 45	O 45	0	0



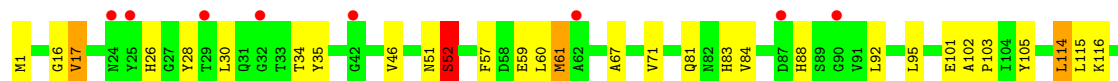
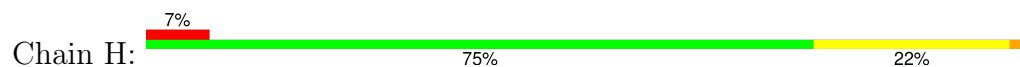
• Molecule 1: Type A flavoprotein fprA

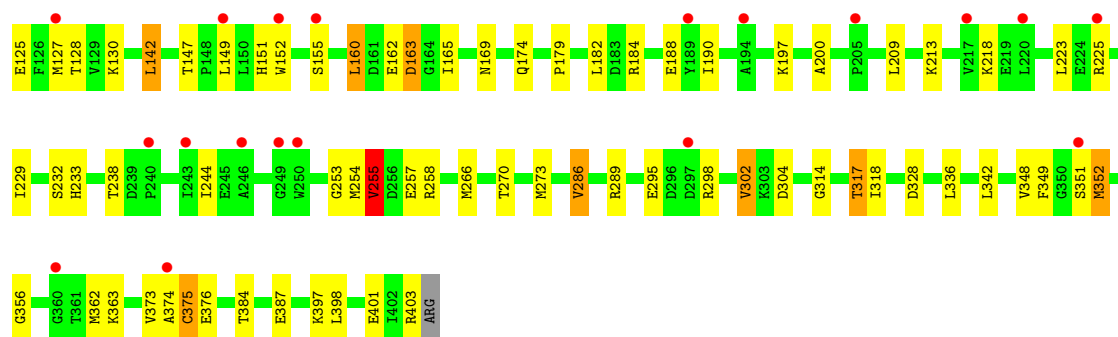


• Molecule 1: Type A flavoprotein fprA

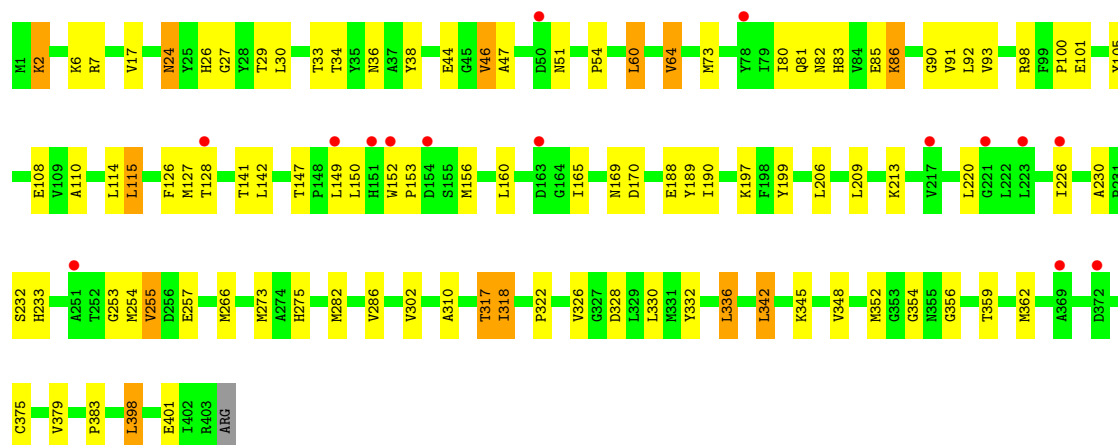
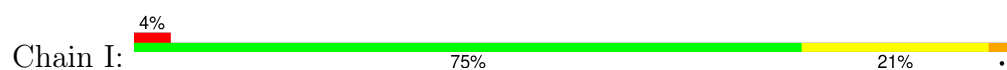


• Molecule 1: Type A flavoprotein fprA

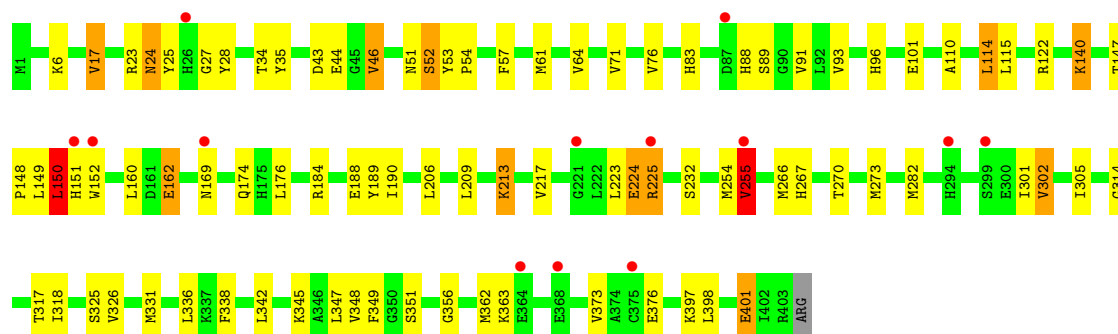
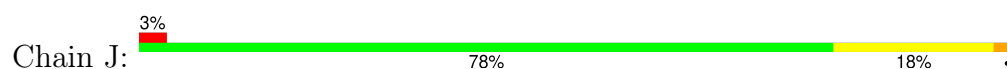




• Molecule 1: Type A flavoprotein fprA



• Molecule 1: Type A flavoprotein fprA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.80Å 123.11Å 135.86Å 90.00° 103.40° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	78.9 (20.00-2.30) 78.7 (20.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	6.60	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.203 , 0.269 0.203 , 0.269	Depositor DCC
R_{free} test set	6932 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25966	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.97 % 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 7.3444e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

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

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	0.70	2/3237 (0.1%)	0.91	5/4386 (0.1%)
1	B	0.69	1/3229 (0.0%)	0.97	6/4375 (0.1%)
1	D	0.66	0/3259	0.92	2/4416 (0.0%)
1	E	0.99	13/3240 (0.4%)	0.97	1/4390 (0.0%)
1	G	0.67	1/3237 (0.0%)	0.94	4/4386 (0.1%)
1	H	0.69	1/3229 (0.0%)	0.92	2/4375 (0.0%)
1	I	0.64	0/3229	0.89	0/4375
1	J	0.70	0/3246	0.93	2/4398 (0.0%)
All	All	0.72	18/25906 (0.1%)	0.93	22/35101 (0.1%)

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	A	0	1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	132	GLY	C-O	21.84	1.53	1.23
1	E	125	GLU	CD-OE2	16.33	1.56	1.25
1	E	43	ASP	CG-OD2	13.89	1.51	1.25
1	A	101	GLU	CD-OE1	10.18	1.44	1.25
1	A	101	GLU	CD-OE2	10.15	1.44	1.25
1	E	130	LYS	CE-NZ	7.87	1.73	1.49
1	G	373	VAL	CA-CB	7.30	1.61	1.53
1	E	133	ASP	N-CA	6.43	1.54	1.46
1	H	125	GLU	CG-CD	6.12	1.67	1.52
1	E	131	THR	CA-C	6.12	1.61	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	136	ASP	C-N	6.02	1.42	1.33
1	E	132	GLY	CA-C	5.87	1.60	1.51
1	E	131	THR	CB-OG1	5.67	1.52	1.43
1	E	133	ASP	CA-CB	5.63	1.62	1.53
1	E	220	LEU	C-N	5.46	1.41	1.33
1	B	373	VAL	CA-CB	5.27	1.60	1.53
1	E	255	VAL	CA-CB	5.16	1.61	1.54
1	E	141	THR	CB-OG1	-5.01	1.35	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	132	GLY	O-C-N	11.12	137.15	122.70
1	D	323	TYR	CA-C-N	7.23	128.88	119.84
1	D	323	TYR	C-N-CA	7.23	128.88	119.84
1	A	254	MET	N-CA-C	6.47	118.13	111.14
1	G	52	SER	N-CA-C	5.90	116.20	107.88
1	A	118	TYR	CA-C-N	5.89	125.57	119.56
1	A	118	TYR	C-N-CA	5.89	125.57	119.56
1	A	255	VAL	N-CA-C	5.86	121.53	109.34
1	B	118	TYR	CA-C-N	5.82	125.50	119.56
1	B	118	TYR	C-N-CA	5.82	125.50	119.56
1	H	52	SER	N-CA-C	5.81	115.77	108.45
1	B	321	GLU	CA-C-N	-5.78	114.31	120.03
1	B	321	GLU	C-N-CA	-5.78	114.31	120.03
1	J	52	SER	N-CA-C	5.75	116.14	108.38
1	G	255	VAL	N-CA-C	5.54	120.87	109.34
1	A	52	SER	N-CA-C	5.45	117.08	108.96
1	B	375	CYS	N-CA-C	5.37	122.23	110.80
1	G	375	CYS	N-CA-C	5.31	122.11	110.80
1	G	86	LYS	N-CA-C	5.17	118.68	112.38
1	H	155	SER	N-CA-C	5.07	117.25	110.35
1	B	161	ASP	N-CA-C	5.03	116.76	111.28
1	J	255	VAL	N-CA-C	5.03	119.80	109.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	GLU	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3166	0	3113	58	0
1	B	3162	0	3111	50	0
1	D	3178	0	3119	49	0
1	E	3168	0	3114	65	0
1	G	3166	0	3113	62	0
1	H	3162	0	3111	54	0
1	I	3162	0	3111	61	0
1	J	3169	0	3115	62	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
3	A	31	0	19	0	0
3	B	31	0	19	0	0
3	D	31	0	19	0	0
3	E	31	0	19	0	0
3	G	31	0	19	0	0
3	H	31	0	19	0	0
3	I	31	0	19	1	0
3	J	31	0	19	0	0
4	D	1	0	0	0	0
4	H	1	0	0	0	0
4	J	2	0	0	0	0
5	A	46	0	0	1	0
5	B	47	0	0	2	0
5	D	57	0	0	3	0
5	E	42	0	0	2	0
5	G	50	0	0	3	0
5	H	45	0	0	3	0
5	I	33	0	0	1	0
5	J	45	0	0	4	0
All	All	25966	0	25059	432	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 9.

All (432) 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:130:LYS:CE	1:E:130:LYS:NZ	1.73	1.47
1:H:266:MET:SD	1:H:318:ILE:HD11	1.98	1.04
1:B:266:MET:SD	1:B:318:ILE:HD11	1.97	1.03
1:A:273:MET:HE1	1:A:351:SER:HB2	1.43	0.96
1:I:266:MET:SD	1:I:318:ILE:HD11	2.05	0.95
1:J:24:ASN:HD21	1:J:27:GLY:H	1.16	0.93
1:J:270:THR:HA	1:J:273:MET:HE3	1.54	0.87
1:J:51:ASN:HD22	1:J:52:SER:H	1.24	0.85
1:G:71:VAL:HG12	1:G:73:MET:HG2	1.58	0.84
1:I:24:ASN:HD21	1:I:27:GLY:H	1.24	0.81
1:A:266:MET:SD	1:A:318:ILE:HD11	2.20	0.81
1:D:317:THR:HG22	1:D:352:MET:HB3	1.63	0.81
1:E:273:MET:HE1	1:E:351:SER:HB2	1.63	0.80
1:G:57:PHE:CE1	1:G:61:MET:HE3	2.17	0.80
1:B:273:MET:HE1	1:B:351:SER:HB2	1.63	0.79
1:D:266:MET:SD	1:D:318:ILE:HD11	2.23	0.78
1:D:67:ALA:O	1:D:71:VAL:HG23	1.83	0.78
1:G:83:HIS:HD2	1:G:169[A]:ASN:HD21	1.33	0.76
1:E:147:THR:HG22	1:E:213:LYS:HE2	1.66	0.76
1:D:266:MET:HG2	1:E:26:HIS:HB2	1.65	0.76
1:E:81:GLN:HE21	1:E:92:LEU:HD13	1.52	0.75
1:G:85:GLU:HG2	1:G:87:ASP:OD1	1.87	0.74
1:G:83:HIS:CD2	1:G:169[A]:ASN:ND2	2.56	0.74
1:J:317:THR:HG21	1:J:356:GLY:HA2	1.70	0.74
1:G:61:MET:HE2	1:G:61:MET:HA	1.68	0.73
1:I:82:ASN:HD22	1:I:156:MET:HG3	1.52	0.73
1:G:83:HIS:CD2	1:G:169[A]:ASN:HD21	2.07	0.73
1:G:51:ASN:HD22	1:G:52:SER:H	1.34	0.72
1:I:317:THR:HG21	1:I:356:GLY:HA2	1.72	0.72
1:A:317:THR:HG21	1:A:356:GLY:HA2	1.71	0.71
1:E:151[A]:HIS:CE1	1:E:169:ASN:HB3	2.24	0.71
1:D:61:MET:HE2	1:D:61:MET:HA	1.71	0.71
1:I:147:THR:HG22	1:I:213:LYS:HE2	1.72	0.71
1:A:26:HIS:HB2	1:B:266:MET:HG2	1.72	0.71
1:H:182:LEU:HD13	1:H:238:THR:HG21	1.73	0.71
1:H:147:THR:HG22	1:H:213:LYS:HE2	1.72	0.71
1:I:83:HIS:HE1	1:I:152:TRP:HB2	1.57	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:257:GLU:HB3	1:G:286:VAL:HG22	1.74	0.69
1:J:24:ASN:C	1:J:24:ASN:HD22	2.00	0.69
1:H:289:ARG:HG3	1:H:304:ASP:OD1	1.92	0.69
1:A:317:THR:HG22	1:A:352:MET:HB3	1.74	0.69
1:H:273:MET:HE1	1:H:351:SER:HB2	1.75	0.69
1:D:83[A]:HIS:HE2	1:D:152:TRP:CG	2.10	0.69
1:G:83:HIS:HD2	1:G:169[A]:ASN:ND2	1.89	0.69
1:H:253:GLY:HA2	5:H:1745:HOH:O	1.92	0.68
1:E:223:LEU:HA	1:E:226:ILE:HD13	1.74	0.68
1:J:61:MET:HE2	1:J:61:MET:HA	1.75	0.68
1:H:179:PRO:HB3	1:J:282:MET:HG2	1.76	0.67
1:B:46:VAL:HG22	1:B:76:VAL:HA	1.77	0.67
1:G:314:GLY:HA2	1:G:349:PHE:O	1.95	0.67
1:A:169[A]:ASN:HD22	1:A:170:ASP:H	1.43	0.67
1:G:71:VAL:CG1	1:G:73:MET:HG2	2.25	0.66
1:E:317:THR:HG21	1:E:356:GLY:HA2	1.78	0.66
1:A:82:ASN:HD22	1:A:156:MET:HG3	1.62	0.65
1:J:83[B]:HIS:CE1	1:J:169:ASN:HB2	2.31	0.65
1:H:190:ILE:HD11	1:J:189:TYR:CZ	2.31	0.65
1:G:169[B]:ASN:HD22	1:G:170:ASP:H	1.45	0.64
1:B:84:VAL:HG12	1:B:114:LEU:HD13	1.77	0.64
1:J:46:VAL:HG22	1:J:76:VAL:HA	1.79	0.64
1:D:162:GLU:HG2	1:D:163:ASP:OD1	1.97	0.64
1:H:142:LEU:HD12	1:H:160:LEU:HD13	1.79	0.64
1:E:266:MET:SD	1:E:318:ILE:HD11	2.38	0.63
1:D:317:THR:HG21	1:D:356:GLY:HA2	1.81	0.63
1:J:162:GLU:H	1:J:162:GLU:CD	2.05	0.63
1:J:83[A]:HIS:HE2	1:J:152:TRP:CG	2.17	0.62
1:I:142:LEU:HD12	1:I:160:LEU:HD13	1.81	0.62
1:B:254:MET:HE2	1:B:254:MET:HA	1.82	0.62
1:A:257:GLU:HB3	1:A:286:VAL:HG22	1.82	0.62
1:I:81:GLN:HE21	1:I:92:LEU:HD13	1.65	0.61
1:G:348:VAL:O	1:G:376:GLU:HA	2.00	0.61
1:I:110:ALA:O	1:I:114:LEU:HB2	2.00	0.61
1:G:26:HIS:HB2	1:H:266:MET:HG2	1.80	0.61
1:J:267:HIS:HB3	5:J:3728:HOH:O	2.01	0.61
1:A:83:HIS:HE1	1:A:152:TRP:CG	2.19	0.60
1:I:332:TYR:O	1:I:336:LEU:HD22	2.01	0.60
1:J:150:LEU:HA	1:J:206:LEU:HD13	1.83	0.60
1:H:17:VAL:HG22	1:H:35:TYR:HD2	1.66	0.60
1:G:46:VAL:HG22	1:G:76:VAL:HA	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:348:VAL:HG13	1:J:362:MET:HE3	1.83	0.60
1:B:352:MET:HG2	1:B:378:GLU:OE2	2.01	0.60
1:E:348:VAL:HG13	1:E:362:MET:HE3	1.84	0.60
1:I:54:PRO:HD3	1:I:90:GLY:HA3	1.84	0.59
1:I:83:HIS:CE1	1:I:152:TRP:HB2	2.36	0.59
1:I:93:VAL:HG12	5:I:2724:HOH:O	2.02	0.59
1:G:254:MET:O	5:G:740:HOH:O	2.17	0.59
1:I:86:LYS:HD2	5:J:3728:HOH:O	2.01	0.59
1:J:17:VAL:HG22	1:J:35:TYR:HD2	1.67	0.59
1:B:189:TYR:CE2	1:E:190:ILE:HD11	2.37	0.59
1:D:57:PHE:CE1	1:D:61:MET:HE3	2.37	0.59
1:E:151[A]:HIS:HE1	1:E:169:ASN:HB3	1.68	0.59
1:J:17:VAL:CG2	1:J:35:TYR:HD2	2.16	0.59
1:H:57:PHE:CZ	1:H:61:MET:HG2	2.38	0.59
1:B:36:ASN:HB2	1:B:232:SER:HA	1.83	0.58
1:D:83[B]:HIS:CE1	1:D:169[B]:ASN:HB2	2.38	0.58
1:E:81:GLN:HE22	1:E:89:SER:HA	1.67	0.58
1:H:254:MET:O	1:H:255:VAL:HG22	2.04	0.58
1:B:57:PHE:CE1	1:B:61:MET:HE3	2.39	0.58
1:H:163:ASP:HB3	1:H:165:ILE:HG13	1.85	0.57
1:B:318:ILE:CD1	1:B:323:TYR:HD1	2.17	0.57
1:H:273:MET:CE	1:H:351:SER:HB2	2.34	0.57
1:G:334:ARG:HH21	1:G:368:GLU:CD	2.12	0.57
1:G:169[B]:ASN:HD22	1:G:170:ASP:N	2.02	0.57
1:G:122:ARG:HE	1:G:123:GLU:N	2.03	0.57
1:B:317:THR:HG23	1:B:352:MET:HB3	1.86	0.56
1:G:51:ASN:ND2	1:G:52:SER:H	2.03	0.56
1:A:317:THR:CG2	1:A:352:MET:HB3	2.36	0.56
1:A:179:PRO:HB3	1:D:282:MET:HG2	1.87	0.56
1:H:270:THR:HA	1:H:273:MET:HE3	1.86	0.56
1:E:24:ASN:HD21	1:E:27:GLY:H	1.54	0.56
1:J:147:THR:HG22	1:J:213:LYS:HD3	1.87	0.56
1:G:315:ALA:HB2	1:G:326:VAL:HG21	1.88	0.56
1:D:317:THR:CG2	1:D:352:MET:HB3	2.36	0.56
1:I:326:VAL:HG12	1:I:330:LEU:HD12	1.87	0.56
1:E:317:THR:HG22	5:E:3717:HOH:O	2.05	0.56
1:I:24:ASN:C	1:I:24:ASN:HD22	2.14	0.55
1:B:348:VAL:O	1:B:376:GLU:HA	2.06	0.55
1:E:83:HIS:HE1	1:E:152:TRP:HB2	1.71	0.55
1:E:254:MET:HA	1:E:254:MET:HE2	1.89	0.55
1:H:57:PHE:CE1	1:H:61:MET:HE3	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:110:ALA:O	1:J:114:LEU:HB2	2.06	0.55
1:G:317:THR:HG23	1:G:352:MET:HB3	1.88	0.55
1:D:397:LYS:HD3	1:D:398:LEU:N	2.21	0.55
1:A:273:MET:CE	1:A:351:SER:HB2	2.28	0.55
1:E:257:GLU:O	1:E:286:VAL:HG13	2.06	0.55
1:H:317:THR:HG23	1:H:352:MET:HB3	1.89	0.55
1:G:61:MET:HE2	1:G:61:MET:CA	2.37	0.54
1:D:83[B]:HIS:CE1	1:D:88:HIS:CD2	2.96	0.54
1:G:222:LEU:HA	1:G:225:ARG:HD2	1.89	0.54
1:B:222:LEU:HA	1:B:225:ARG:HD2	1.90	0.54
1:D:273:MET:CE	1:D:351:SER:HB2	2.38	0.54
1:A:319:TYR:O	1:A:320:ASP:HB2	2.07	0.54
1:E:110:ALA:HB2	1:E:154:ASP:HB2	1.89	0.54
1:E:130:LYS:NZ	1:E:130:LYS:CD	2.66	0.54
1:G:21:ASP:OD2	1:I:275:HIS:CE1	2.61	0.54
1:J:57:PHE:CE1	1:J:61:MET:HE3	2.42	0.54
1:J:83[B]:HIS:ND1	1:J:169:ASN:HB2	2.23	0.54
1:A:46:VAL:HG23	1:A:76:VAL:HA	1.88	0.54
1:I:114:LEU:HD23	1:I:126:PHE:HE2	1.73	0.53
1:D:93:VAL:HG12	5:D:2742:HOH:O	2.08	0.53
1:D:358:ALA:HB3	5:D:2715:HOH:O	2.07	0.53
1:I:26:HIS:HB2	1:J:266:MET:HG2	1.90	0.53
1:J:51:ASN:HD22	1:J:52:SER:N	2.00	0.53
1:A:273:MET:HE1	1:A:351:SER:CB	2.29	0.53
1:E:83:HIS:HE1	1:E:152:TRP:CG	2.27	0.53
1:B:257:GLU:HB3	1:B:286:VAL:HG22	1.90	0.53
1:J:96:HIS:HD2	5:J:3707:HOH:O	1.91	0.53
1:B:81:GLN:HG3	1:B:114:LEU:HD21	1.91	0.53
1:G:160:LEU:HD23	1:G:165:ILE:HD12	1.91	0.53
1:H:257:GLU:HB3	1:H:286:VAL:HG22	1.91	0.52
1:A:346:ALA:HB3	1:A:373:VAL:HB	1.90	0.52
1:I:273:MET:CE	1:I:379:VAL:HB	2.40	0.52
1:J:51:ASN:ND2	1:J:52:SER:H	2.02	0.52
1:E:348:VAL:HG12	1:E:359:THR:HG22	1.91	0.52
1:H:190:ILE:HD11	1:J:189:TYR:OH	2.08	0.52
1:E:83:HIS:CE1	1:E:152:TRP:HB2	2.45	0.52
1:I:322:PRO:HG2	1:J:331:MET:SD	2.50	0.52
1:D:217:VAL:HG13	1:D:222:LEU:HB2	1.91	0.52
1:A:348:VAL:O	1:A:376:GLU:HA	2.10	0.51
1:E:146:GLU:O	1:E:213:LYS:NZ	2.43	0.51
1:G:216:GLU:HA	1:G:219:GLU:OE1	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:24:ASN:HD21	1:J:27:GLY:N	1.96	0.51
1:I:160:LEU:HD23	1:I:165:ILE:HD12	1.92	0.51
1:D:60:LEU:O	1:D:64:VAL:HG13	2.11	0.51
1:G:21:ASP:OD2	1:I:275:HIS:HE1	1.94	0.51
1:I:46:VAL:HG13	1:I:73:MET:HE2	1.93	0.51
1:E:147:THR:HG22	1:E:213:LYS:CE	2.40	0.51
1:A:61:MET:HA	1:A:64:VAL:HG22	1.93	0.51
1:B:66:ASP:O	1:B:69:GLN:HB2	2.11	0.51
1:I:149:LEU:O	1:I:206:LEU:HD22	2.11	0.51
1:E:257:GLU:C	1:E:286:VAL:HG13	2.36	0.51
1:G:119:PRO:O	1:G:122:ARG:HG3	2.11	0.51
1:J:224:GLU:HG2	1:J:225:ARG:HG3	1.93	0.51
1:B:241:MET:O	1:B:245:GLU:HG3	2.11	0.50
1:H:348:VAL:O	1:H:376:GLU:HA	2.11	0.50
1:E:169:ASN:HD22	1:E:170:ASP:H	1.59	0.50
1:B:282:MET:HE1	1:E:18:LEU:HD11	1.94	0.50
1:E:273:MET:HE1	1:E:351:SER:CB	2.40	0.50
1:D:142:LEU:HD23	1:D:158:THR:HG21	1.93	0.50
1:A:229:ILE:HD11	1:A:244:ILE:HD11	1.94	0.50
1:B:21:ASP:OD2	1:E:275:HIS:CE1	2.64	0.50
1:B:81:GLN:HE21	1:B:92:LEU:HD13	1.77	0.50
1:A:147:THR:HG22	1:A:213:LYS:HE2	1.94	0.50
1:B:319:TYR:O	1:B:320:ASP:HB2	2.12	0.50
1:D:13:TYR:HE1	1:D:70:GLN:NE2	2.09	0.50
1:E:315:ALA:HB2	1:E:326:VAL:HG21	1.94	0.50
1:A:266:MET:HG2	1:B:26:HIS:HB2	1.93	0.50
1:B:266:MET:SD	1:B:318:ILE:CD1	2.87	0.50
1:G:363:LYS:HE3	1:G:373:VAL:HG22	1.93	0.50
1:J:150:LEU:HG	1:J:150:LEU:O	2.12	0.50
1:H:317:THR:HG22	5:H:1713:HOH:O	2.11	0.50
1:E:24:ASN:ND2	1:E:27:GLY:H	2.10	0.49
1:G:151:HIS:HD2	5:G:709:HOH:O	1.95	0.49
1:J:88:HIS:CE1	1:J:232[B]:SER:HB3	2.46	0.49
1:H:348:VAL:HG13	1:H:362:MET:HE3	1.94	0.49
1:A:83:HIS:HE1	1:A:152:TRP:CD2	2.30	0.49
1:B:1:MET:HE2	1:B:3:ALA:HB2	1.93	0.49
1:G:330:LEU:HD13	1:G:365:LEU:HB2	1.95	0.49
1:D:273:MET:HE1	1:D:351:SER:HB2	1.93	0.49
1:A:202:LEU:O	1:B:319:TYR:OH	2.20	0.49
1:I:152:TRP:HB3	1:I:153:PRO:HD2	1.95	0.49
1:A:17:VAL:HG11	1:A:52:SER:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:273:MET:O	1:E:277:ILE:HG13	2.12	0.49
1:A:196:ARG:HD3	1:A:307:GLU:HG3	1.95	0.49
1:A:46:VAL:HG21	1:A:75:ARG:O	2.13	0.49
1:E:83:HIS:CE1	1:E:151[A]:HIS:HD2	2.31	0.49
1:B:84:VAL:HG13	1:B:154:ASP:OD2	2.13	0.49
1:B:314:GLY:HA2	1:B:349:PHE:O	2.13	0.49
1:D:397:LYS:HD3	1:D:397:LYS:C	2.38	0.49
1:E:38:TYR:CZ	1:E:230:ALA:HB1	2.48	0.49
1:I:199:TYR:C	1:I:199:TYR:CD2	2.91	0.49
1:H:84:VAL:HG12	1:H:114:LEU:HD22	1.95	0.48
1:J:266:MET:SD	1:J:318:ILE:HD11	2.52	0.48
1:J:348:VAL:CG1	1:J:362:MET:HE3	2.44	0.48
1:J:254:MET:HA	1:J:254:MET:HE2	1.94	0.48
1:A:169[A]:ASN:HD22	1:A:170:ASP:N	2.10	0.48
1:H:374:ALA:O	1:H:375:CYS:HB2	2.14	0.48
1:E:160:LEU:HD23	1:E:165:ILE:HD12	1.96	0.48
1:E:273:MET:CE	1:E:351:SER:HB2	2.37	0.48
1:D:58:ASP:HB2	5:D:2705:HOH:O	2.13	0.48
1:E:61:MET:O	1:E:65:GLU:HG3	2.14	0.48
1:H:200:ALA:HB1	1:H:302:VAL:HG12	1.96	0.48
1:E:8:ILE:HG21	1:E:236:ILE:HD13	1.95	0.48
1:J:348:VAL:O	1:J:376:GLU:HA	2.12	0.48
1:B:152:TRP:HB3	1:B:154:ASP:OD1	2.14	0.47
1:E:200:ALA:HB2	1:E:306:LEU:HD22	1.95	0.47
1:G:46:VAL:HG12	1:G:73:MET:HE2	1.96	0.47
1:A:326:VAL:HG12	1:A:330:LEU:HD12	1.96	0.47
1:G:6:LYS:HE3	1:G:181:ARG:HB2	1.96	0.47
1:H:83:HIS:CD2	1:H:169:ASN:HD21	2.32	0.47
1:I:273:MET:HE1	1:I:379:VAL:HB	1.96	0.47
1:J:24:ASN:C	1:J:24:ASN:ND2	2.70	0.47
1:E:334:ARG:O	1:E:337:LYS:NZ	2.47	0.47
1:J:53:TYR:CG	1:J:54:PRO:HD2	2.49	0.47
1:D:24:ASN:C	1:D:24:ASN:HD22	2.23	0.47
1:H:28:TYR:CE2	1:H:197:LYS:HE2	2.50	0.47
1:H:67:ALA:O	1:H:71:VAL:HG23	2.15	0.47
1:I:266:MET:SD	1:I:318:ILE:CD1	2.92	0.47
1:D:259:VAL:HG22	1:D:310:ALA:HB3	1.96	0.47
1:D:294:HIS:O	1:D:294:HIS:ND1	2.45	0.47
1:E:53:TYR:CG	1:E:54:PRO:HD2	2.50	0.47
1:H:273:MET:HE1	1:H:351:SER:CB	2.44	0.47
1:J:345:LYS:HD2	1:J:401:GLU:OE2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:MET:HG2	1:D:179:PRO:HB3	1.96	0.46
1:B:181:ARG:NH2	5:B:1742:HOH:O	2.42	0.46
1:A:83:HIS:CE1	1:A:152:TRP:HB2	2.50	0.46
1:A:269:SER:O	1:A:273:MET:HE3	2.14	0.46
1:B:61:MET:HE2	1:B:61:MET:HA	1.97	0.46
1:H:363:LYS:O	1:H:373:VAL:HG11	2.15	0.46
1:J:301:ILE:O	1:J:305:ILE:HG13	2.15	0.46
1:I:38:TYR:CZ	1:I:230:ALA:HB1	2.50	0.46
1:H:88:HIS:CE1	1:H:232:SER:HB2	2.50	0.46
1:I:169:ASN:ND2	1:I:170:ASP:H	2.12	0.46
1:J:88:HIS:CE1	1:J:232[A]:SER:HB2	2.49	0.46
1:A:46:VAL:CG2	1:A:75:ARG:O	2.64	0.46
1:G:223:LEU:HA	1:G:226:ILE:HD12	1.97	0.46
1:J:34:THR:HG23	1:J:176:LEU:O	2.16	0.46
1:B:173:GLY:C	1:B:174:GLN:HG3	2.41	0.46
1:G:199:TYR:HA	1:G:203:ILE:HG12	1.96	0.46
1:B:363:LYS:HG2	1:B:373:VAL:HG21	1.98	0.46
1:G:71:VAL:CG1	1:G:73:MET:CG	2.93	0.46
1:G:179:PRO:HB3	1:I:282:MET:HG2	1.98	0.46
1:I:51:ASN:HD22	1:I:91:VAL:HG22	1.81	0.46
1:J:184:ARG:NH1	5:J:3722:HOH:O	2.30	0.46
1:D:317:THR:HG22	1:D:352:MET:CB	2.42	0.46
1:I:310:ALA:HB1	1:I:398:LEU:HD22	1.98	0.46
1:A:271:ARG:NH1	5:A:741:HOH:O	2.48	0.46
1:G:8:ILE:HG21	1:G:236:ILE:HD13	1.98	0.45
1:H:295:GLU:HB3	1:J:23:ARG:HG3	1.98	0.45
1:J:189:TYR:CD2	1:J:189:TYR:C	2.94	0.45
1:E:374:ALA:O	1:E:375:CYS:HB2	2.17	0.45
1:G:380:TYR:CD1	1:H:116:LYS:HG2	2.51	0.45
1:I:348:VAL:HG12	1:I:359:THR:HG22	1.99	0.45
1:J:148:PRO:O	1:J:149:LEU:C	2.60	0.45
1:A:161:ASP:C	1:A:163:ASP:H	2.23	0.45
1:B:273:MET:CE	1:B:351:SER:HB2	2.39	0.45
1:A:322:PRO:O	1:A:323:TYR:C	2.60	0.45
1:D:310:ALA:HB1	1:D:398:LEU:HD22	1.98	0.45
1:I:36:ASN:HB2	1:I:232:SER:HA	1.99	0.45
1:I:60:LEU:O	1:I:64:VAL:HG13	2.17	0.45
1:G:162:GLU:CD	1:G:162:GLU:H	2.24	0.45
1:G:318:ILE:O	1:G:319:TYR:C	2.59	0.45
1:H:105:TYR:CE1	1:H:127:MET:HG2	2.52	0.45
1:I:33:THR:OG1	1:I:34:THR:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:VAL:HG12	1:D:114:LEU:HD13	1.99	0.45
1:E:17:VAL:HG22	1:E:35:TYR:HD2	1.82	0.45
1:H:273:MET:HE1	1:H:351:SER:N	2.32	0.45
1:B:150:LEU:HA	1:B:151:HIS:HA	1.75	0.45
1:I:348:VAL:CG1	1:I:362:MET:HE3	2.46	0.45
1:A:21:ASP:OD1	1:D:263:TYR:OH	2.29	0.44
1:H:317:THR:HG21	1:H:356:GLY:HA2	1.99	0.44
1:I:29:THR:O	1:I:197:LYS:NZ	2.49	0.44
1:J:169:ASN:HA	1:J:232[B]:SER:OG	2.17	0.44
1:J:273:MET:HE1	1:J:351:SER:N	2.32	0.44
1:B:184:ARG:NH1	5:B:1706:HOH:O	2.50	0.44
1:A:8:ILE:HG21	1:A:236:ILE:HD13	2.00	0.44
1:G:82:ASN:HD22	1:G:156:MET:HG3	1.81	0.44
1:I:254:MET:HE2	1:I:254:MET:HA	2.00	0.44
1:E:348:VAL:O	1:E:376:GLU:HA	2.18	0.44
1:J:363:LYS:HG3	1:J:373:VAL:HG11	2.00	0.44
1:A:273:MET:HG2	1:A:391:CYS:SG	2.58	0.44
1:G:258:ARG:HB2	1:G:258:ARG:NH1	2.32	0.44
1:H:229:ILE:HD11	1:H:244:ILE:HD11	2.00	0.44
1:B:83:HIS:HE1	1:B:152:TRP:CE3	2.35	0.44
1:H:60:LEU:HD23	1:H:61:MET:HE2	1.99	0.44
1:H:81:GLN:HE21	1:H:92:LEU:HD13	1.83	0.44
1:A:150:LEU:HA	1:A:206:LEU:HD13	2.00	0.43
1:H:17:VAL:HB	1:H:59:GLU:CD	2.43	0.43
1:A:317:THR:HB	1:A:358:ALA:HB2	2.00	0.43
1:D:142:LEU:N	1:D:142:LEU:HD12	2.32	0.43
1:E:53:TYR:CD1	1:E:54:PRO:HD2	2.53	0.43
1:G:83:HIS:HE1	1:G:152:TRP:CD2	2.35	0.43
1:G:262:ILE:O	1:G:313:LEU:HA	2.18	0.43
1:H:83:HIS:HD2	1:H:169:ASN:HD21	1.66	0.43
1:I:34:THR:O	1:I:233:HIS:ND1	2.50	0.43
1:J:51:ASN:HD21	1:J:89:SER:C	2.26	0.43
1:H:384:THR:HG23	1:H:387:GLU:OE1	2.18	0.43
1:B:140:LYS:HG2	1:B:160:LEU:HD11	2.00	0.43
1:G:54:PRO:HD3	1:G:90:GLY:HA3	2.00	0.43
1:G:51:ASN:ND2	1:G:91:VAL:H	2.16	0.43
1:H:51:ASN:HD22	1:H:52:SER:H	1.65	0.43
1:A:291:TYR:OH	1:A:304:ASP:OD1	2.23	0.43
1:D:38:TYR:CZ	1:D:230:ALA:HB1	2.54	0.43
1:E:57:PHE:CE1	1:E:61:MET:HE3	2.53	0.43
1:I:85:GLU:OE2	1:J:267:HIS:NE2	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:HIS:HB3	1:B:86:LYS:HD2	2.01	0.43
1:D:348:VAL:O	1:D:376:GLU:HA	2.18	0.43
1:E:102:ALA:HA	1:E:103:PRO:HD2	1.94	0.43
1:G:36:ASN:HB2	1:G:232:SER:HA	1.99	0.43
1:A:189:TYR:C	1:A:189:TYR:CD2	2.97	0.43
1:A:314:GLY:HA2	1:A:349:PHE:O	2.18	0.43
1:D:226:ILE:HG23	1:D:226:ILE:O	2.18	0.43
1:H:83:HIS:HE1	1:H:152:TRP:CG	2.36	0.43
1:H:298:ARG:NH1	1:H:328:ASP:OD1	2.51	0.43
1:I:257:GLU:HB3	1:I:286:VAL:HG22	2.01	0.42
1:A:281:ALA:HA	1:A:399:ALA:HB2	2.02	0.42
1:B:213:LYS:O	1:B:217:VAL:HG23	2.19	0.42
1:E:131:THR:H	1:E:146:GLU:HG3	1.84	0.42
1:I:345:LYS:HD2	1:I:401:GLU:HG2	2.01	0.42
1:J:213:LYS:O	1:J:217:VAL:HG23	2.19	0.42
1:D:189:TYR:CD2	1:D:189:TYR:C	2.97	0.42
1:I:354:GLY:N	3:I:2702:FMN:O2	2.51	0.42
1:A:131:THR:HG23	1:A:145:LEU:HD12	2.01	0.42
1:G:8:ILE:HG21	1:G:236:ILE:CD1	2.50	0.42
1:H:403:ARG:HD2	5:H:1718:HOH:O	2.18	0.42
1:I:253:GLY:O	1:I:342:LEU:HD12	2.20	0.42
1:J:71:VAL:HG12	1:J:71:VAL:O	2.18	0.42
1:A:17:VAL:HG13	1:A:35:TYR:HB2	2.01	0.42
1:E:61:MET:HB3	5:E:3705:HOH:O	2.19	0.42
1:E:67:ALA:O	1:E:71:VAL:HG23	2.19	0.42
1:B:254:MET:HA	1:B:254:MET:CE	2.48	0.42
1:B:277:ILE:HG13	1:B:391:CYS:HB3	2.01	0.42
1:B:162:GLU:CD	1:B:162:GLU:H	2.27	0.42
1:D:400:ALA:HA	1:D:403:ARG:HG3	2.01	0.42
1:H:363:LYS:HD3	1:H:376:GLU:OE2	2.20	0.42
1:I:47:ALA:HB1	1:I:80:ILE:HD12	2.02	0.42
1:I:83:HIS:HB2	1:I:169:ASN:OD1	2.19	0.42
1:E:343:THR:HG22	1:E:372:ASP:HB2	2.01	0.42
1:I:100:PRO:HG2	1:I:101:GLU:OE1	2.20	0.42
1:E:358:ALA:O	1:E:362:MET:HG3	2.20	0.42
1:G:190:ILE:HD11	1:I:189:TYR:CE2	2.54	0.42
1:G:337:LYS:NZ	5:G:751:HOH:O	2.52	0.42
1:H:83:HIS:CD2	1:H:169:ASN:ND2	2.87	0.42
1:I:328:ASP:OD1	1:J:325:SER:HA	2.20	0.42
1:E:61:MET:HA	1:E:64:VAL:HG22	2.01	0.41
1:H:314:GLY:HA2	1:H:349:PHE:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:THR:HB	1:A:150:LEU:HB3	2.01	0.41
1:D:51:ASN:OD1	1:D:81:GLN:NE2	2.54	0.41
1:G:317:THR:HG22	1:G:358:ALA:HB3	2.02	0.41
1:I:115:LEU:HD13	1:I:115:LEU:HA	1.85	0.41
1:J:363:LYS:HG3	1:J:373:VAL:HG21	2.00	0.41
1:A:27:GLY:HA3	1:B:323:TYR:OH	2.21	0.41
1:A:201:ASN:OD1	1:A:299:SER:HA	2.20	0.41
1:D:115:LEU:HD12	1:D:115:LEU:HA	1.94	0.41
1:E:322:PRO:O	1:E:323:TYR:C	2.63	0.41
1:J:140:LYS:HG2	1:J:160:LEU:HD11	2.01	0.41
1:D:147:THR:HB	1:D:150:LEU:HB2	2.02	0.41
1:G:59:GLU:OE1	1:G:63:ARG:NH2	2.49	0.41
1:H:102:ALA:HA	1:H:103:PRO:HD3	1.95	0.41
1:H:258:ARG:HE	1:H:289:ARG:NH1	2.18	0.41
1:I:379:VAL:HG11	1:I:383:PRO:HB3	2.03	0.41
1:J:53:TYR:CD2	1:J:54:PRO:HD2	2.56	0.41
1:D:46:VAL:HG22	1:D:76:VAL:HA	2.01	0.41
1:E:26:HIS:CD2	1:E:26:HIS:O	2.74	0.41
1:H:16:GLY:HA3	1:H:35:TYR:O	2.21	0.41
1:J:25:TYR:O	1:J:28:TYR:HB3	2.21	0.41
1:E:36:ASN:HB2	1:E:232:SER:HA	2.03	0.41
1:E:136:ASP:HA	1:E:141:THR:HG22	2.03	0.41
1:G:317:THR:HG22	1:G:358:ALA:CB	2.51	0.41
1:I:83:HIS:CD2	1:I:169:ASN:HD21	2.39	0.41
1:I:114:LEU:HD12	1:I:114:LEU:HA	1.98	0.41
1:I:190:ILE:HD13	1:I:190:ILE:HA	1.86	0.41
1:A:81:GLN:HE21	1:A:92:LEU:HD13	1.85	0.41
1:A:263:TYR:HA	1:A:314:GLY:O	2.21	0.41
1:A:298:ARG:NH1	1:A:328:ASP:OD1	2.53	0.41
1:B:83:HIS:CD2	1:B:169:ASN:ND2	2.89	0.41
1:B:145:LEU:HD11	1:B:216:GLU:OE2	2.21	0.41
1:B:326:VAL:HG13	1:B:330:LEU:HD12	2.03	0.41
1:D:51:ASN:HD22	1:D:52:SER:H	1.67	0.41
1:E:51:ASN:ND2	1:E:91:VAL:H	2.18	0.41
1:G:51:ASN:HD21	1:G:89:SER:C	2.28	0.41
1:G:69:GLN:HE21	1:G:69:GLN:HB2	1.63	0.41
1:I:105:TYR:CE1	1:I:127:MET:HG2	2.56	0.41
1:I:152:TRP:HB3	1:I:153:PRO:CD	2.51	0.41
1:J:51:ASN:ND2	1:J:91:VAL:H	2.19	0.41
1:A:228:MET:HE2	1:A:238:THR:HG22	2.02	0.41
1:B:83:HIS:HE1	1:B:152:TRP:CD2	2.39	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:THR:OG1	1:D:34:THR:N	2.54	0.41
1:D:157:PHE:CD1	1:D:168:SER:HA	2.56	0.41
1:D:315:ALA:HB2	1:D:326:VAL:HG21	2.03	0.41
1:E:191:LEU:HD21	1:E:237:TRP:CZ3	2.55	0.41
1:G:392:PHE:C	1:G:392:PHE:CD2	2.99	0.41
1:B:273:MET:HE1	1:B:351:SER:CB	2.41	0.40
1:J:302:VAL:HG13	1:J:338:PHE:HZ	1.86	0.40
1:G:266:MET:SD	1:G:318:ILE:HD11	2.61	0.40
1:G:392:PHE:CD1	1:I:2:LYS:HB3	2.56	0.40
1:H:34:THR:O	1:H:233:HIS:ND1	2.50	0.40
1:I:85:GLU:HG2	1:I:152:TRP:CH2	2.57	0.40
1:G:147:THR:HG22	1:G:213:LYS:HD3	2.02	0.40
1:J:314:GLY:HA2	1:J:349:PHE:O	2.22	0.40
1:A:363:LYS:NZ	1:A:373:VAL:O	2.55	0.40
1:A:392:PHE:CD2	1:A:392:PHE:C	2.99	0.40
1:D:322:PRO:HG2	1:E:331:MET:SD	2.61	0.40
1:E:399:ALA:O	1:E:402:ILE:HG13	2.21	0.40
1:J:273:MET:CE	1:J:351:SER:HB2	2.50	0.40
1:A:82:ASN:O	1:A:155:SER:HA	2.21	0.40
1:A:169[B]:ASN:OD1	1:A:170:ASP:N	2.55	0.40
1:B:189:TYR:CZ	1:E:190:ILE:HD11	2.57	0.40
1:E:12:VAL:HG21	1:E:165:ILE:CD1	2.52	0.40
1:E:353:GLY:O	1:E:380:TYR:HE2	2.05	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	402/404 (100%)	384 (96%)	16 (4%)	2 (0%)	24	31
1	B	401/404 (99%)	382 (95%)	16 (4%)	3 (1%)	18	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	404/404 (100%)	388 (96%)	14 (4%)	2 (0%)	24	31
1	E	402/404 (100%)	377 (94%)	22 (6%)	3 (1%)	18	23
1	G	402/404 (100%)	386 (96%)	14 (4%)	2 (0%)	24	31
1	H	401/404 (99%)	381 (95%)	17 (4%)	3 (1%)	18	23
1	I	401/404 (99%)	374 (93%)	24 (6%)	3 (1%)	18	23
1	J	403/404 (100%)	388 (96%)	13 (3%)	2 (0%)	24	31
All	All	3216/3232 (100%)	3060 (95%)	136 (4%)	20 (1%)	21	27

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	VAL
1	B	375	CYS
1	D	255	VAL
1	J	150	LEU
1	B	255	VAL
1	E	255	VAL
1	G	255	VAL
1	G	375	CYS
1	H	255	VAL
1	I	255	VAL
1	J	255	VAL
1	B	254	MET
1	E	149	LEU
1	H	26	HIS
1	A	375	CYS
1	D	226	ILE
1	H	375	CYS
1	I	86	LYS
1	I	375	CYS
1	E	226	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	336/336 (100%)	313 (93%)	23 (7%)	14	20
1	B	335/336 (100%)	298 (89%)	37 (11%)	6	7
1	D	338/336 (101%)	312 (92%)	26 (8%)	12	16
1	E	336/336 (100%)	306 (91%)	30 (9%)	9	12
1	G	336/336 (100%)	304 (90%)	32 (10%)	8	10
1	H	335/336 (100%)	300 (90%)	35 (10%)	7	8
1	I	335/336 (100%)	307 (92%)	28 (8%)	10	14
1	J	337/336 (100%)	304 (90%)	33 (10%)	7	10
All	All	2688/2688 (100%)	2444 (91%)	244 (9%)	9	11

All (244) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	ASP
1	A	17	VAL
1	A	30	LEU
1	A	31	GLN
1	A	71	VAL
1	A	109	VAL
1	A	114	LEU
1	A	115	LEU
1	A	120	SER
1	A	128	THR
1	A	140	LYS
1	A	150	LEU
1	A	151	HIS
1	A	188	GLU
1	A	317	THR
1	A	336	LEU
1	A	337	LYS
1	A	342	LEU
1	A	348	VAL
1	A	373	VAL
1	A	378	GLU
1	A	398	LEU
1	B	17	VAL
1	B	24	ASN
1	B	30	LEU
1	B	46	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	60	LEU
1	B	64	VAL
1	B	69	GLN
1	B	93	VAL
1	B	94	GLU
1	B	114	LEU
1	B	115	LEU
1	B	122	ARG
1	B	123	GLU
1	B	131	THR
1	B	134	VAL
1	B	142	LEU
1	B	151	HIS
1	B	162	GLU
1	B	174	GLN
1	B	184	ARG
1	B	188	GLU
1	B	209	LEU
1	B	223	LEU
1	B	225	ARG
1	B	255	VAL
1	B	282	MET
1	B	286	VAL
1	B	300	GLU
1	B	302	VAL
1	B	317	THR
1	B	326	VAL
1	B	336	LEU
1	B	342	LEU
1	B	373	VAL
1	B	375	CYS
1	B	397	LYS
1	B	398	LEU
1	D	2	LYS
1	D	17	VAL
1	D	24	ASN
1	D	46	VAL
1	D	64	VAL
1	D	69	GLN
1	D	71	VAL
1	D	114	LEU
1	D	115	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	150	LEU
1	D	162	GLU
1	D	163	ASP
1	D	174	GLN
1	D	188	GLU
1	D	209	LEU
1	D	226	ILE
1	D	302	VAL
1	D	318	ILE
1	D	336	LEU
1	D	342	LEU
1	D	352	MET
1	D	355	ASN
1	D	373	VAL
1	D	397	LYS
1	D	398	LEU
1	D	402	ILE
1	E	6	LYS
1	E	17	VAL
1	E	30	LEU
1	E	31	GLN
1	E	46	VAL
1	E	101	GLU
1	E	114	LEU
1	E	115	LEU
1	E	125	GLU
1	E	128	THR
1	E	134	VAL
1	E	142	LEU
1	E	151[A]	HIS
1	E	151[B]	HIS
1	E	159	LEU
1	E	162	GLU
1	E	174	GLN
1	E	184	ARG
1	E	188	GLU
1	E	218	LYS
1	E	220	LEU
1	E	226	ILE
1	E	255	VAL
1	E	302	VAL
1	E	317	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	336	LEU
1	E	337	LYS
1	E	342	LEU
1	E	398	LEU
1	E	401	GLU
1	G	6	LYS
1	G	7	ARG
1	G	9	SER
1	G	17	VAL
1	G	30	LEU
1	G	31	GLN
1	G	46	VAL
1	G	64	VAL
1	G	71	VAL
1	G	73	MET
1	G	101	GLU
1	G	109	VAL
1	G	112	LYS
1	G	114	LEU
1	G	122	ARG
1	G	141	THR
1	G	142	LEU
1	G	150	LEU
1	G	151	HIS
1	G	162	GLU
1	G	174	GLN
1	G	188	GLU
1	G	225	ARG
1	G	255	VAL
1	G	286	VAL
1	G	302	VAL
1	G	317	THR
1	G	336	LEU
1	G	342	LEU
1	G	352	MET
1	G	373	VAL
1	G	398	LEU
1	H	1	MET
1	H	17	VAL
1	H	30	LEU
1	H	46	VAL
1	H	52	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	61	MET
1	H	95	LEU
1	H	101	GLU
1	H	114	LEU
1	H	115	LEU
1	H	128	THR
1	H	130	LYS
1	H	142	LEU
1	H	149	LEU
1	H	151	HIS
1	H	160	LEU
1	H	162	GLU
1	H	163	ASP
1	H	174	GLN
1	H	184	ARG
1	H	188	GLU
1	H	209	LEU
1	H	218	LYS
1	H	223	LEU
1	H	225	ARG
1	H	255	VAL
1	H	286	VAL
1	H	302	VAL
1	H	317	THR
1	H	336	LEU
1	H	342	LEU
1	H	352	MET
1	H	397	LYS
1	H	398	LEU
1	H	401	GLU
1	I	2	LYS
1	I	6	LYS
1	I	7	ARG
1	I	17	VAL
1	I	24	ASN
1	I	30	LEU
1	I	44	GLU
1	I	46	VAL
1	I	60	LEU
1	I	64	VAL
1	I	98	ARG
1	I	108	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	115	LEU
1	I	128	THR
1	I	141	THR
1	I	150	LEU
1	I	188	GLU
1	I	209	LEU
1	I	220	LEU
1	I	226	ILE
1	I	255	VAL
1	I	302	VAL
1	I	317	THR
1	I	318	ILE
1	I	336	LEU
1	I	342	LEU
1	I	352	MET
1	I	398	LEU
1	J	6	LYS
1	J	17	VAL
1	J	24	ASN
1	J	43	ASP
1	J	44	GLU
1	J	46	VAL
1	J	64	VAL
1	J	93	VAL
1	J	101	GLU
1	J	114	LEU
1	J	115	LEU
1	J	122	ARG
1	J	140	LYS
1	J	150	LEU
1	J	151	HIS
1	J	162	GLU
1	J	174	GLN
1	J	188	GLU
1	J	190	ILE
1	J	209	LEU
1	J	213	LYS
1	J	223	LEU
1	J	224	GLU
1	J	225	ARG
1	J	255	VAL
1	J	302	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	326	VAL
1	J	336	LEU
1	J	342	LEU
1	J	347	LEU
1	J	397	LYS
1	J	398	LEU
1	J	401	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	51	ASN
1	A	70	GLN
1	A	81	GLN
1	A	82	ASN
1	A	83	HIS
1	A	96	HIS
1	A	151	HIS
1	A	275	HIS
1	A	355	ASN
1	B	26	HIS
1	B	31	GLN
1	B	51	ASN
1	B	70	GLN
1	B	81	GLN
1	B	82	ASN
1	B	83	HIS
1	B	227	GLN
1	B	267	HIS
1	B	275	HIS
1	B	355	ASN
1	D	24	ASN
1	D	26	HIS
1	D	51	ASN
1	D	70	GLN
1	D	81	GLN
1	D	82	ASN
1	D	96	HIS
1	D	275	HIS
1	E	24	ASN
1	E	26	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	31	GLN
1	E	51	ASN
1	E	81	GLN
1	E	169	ASN
1	E	275	HIS
1	E	355	ASN
1	G	24	ASN
1	G	26	HIS
1	G	51	ASN
1	G	69	GLN
1	G	81	GLN
1	G	82	ASN
1	G	83	HIS
1	G	151	HIS
1	G	267	HIS
1	G	275	HIS
1	G	339	ASN
1	G	355	ASN
1	H	26	HIS
1	H	51	ASN
1	H	81	GLN
1	H	82	ASN
1	H	83	HIS
1	H	169	ASN
1	H	275	HIS
1	H	294	HIS
1	I	24	ASN
1	I	26	HIS
1	I	31	GLN
1	I	51	ASN
1	I	81	GLN
1	I	82	ASN
1	I	83	HIS
1	I	169	ASN
1	I	275	HIS
1	J	24	ASN
1	J	31	GLN
1	J	51	ASN
1	J	81	GLN
1	J	82	ASN
1	J	96	HIS
1	J	151	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	275	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 20 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	FMN	E	3701	-	33,33,33	1.10	2 (6%)	48,50,50	1.30	7 (14%)
3	FMN	A	701	-	33,33,33	1.12	2 (6%)	48,50,50	1.38	7 (14%)
3	FMN	D	2701	-	33,33,33	1.12	2 (6%)	48,50,50	1.41	9 (18%)
3	FMN	J	3702	-	33,33,33	1.19	3 (9%)	48,50,50	1.31	7 (14%)
3	FMN	G	702	-	33,33,33	1.08	2 (6%)	48,50,50	1.48	8 (16%)
3	FMN	H	1702	-	33,33,33	1.13	2 (6%)	48,50,50	1.38	7 (14%)
3	FMN	I	2702	-	33,33,33	1.15	2 (6%)	48,50,50	1.26	6 (12%)
3	FMN	B	1701	-	33,33,33	1.08	2 (6%)	48,50,50	1.57	13 (27%)

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	E	3701	-	-	5/18/18/18	0/3/3/3
3	FMN	A	701	-	-	2/18/18/18	0/3/3/3
3	FMN	D	2701	-	-	3/18/18/18	0/3/3/3
3	FMN	J	3702	-	-	3/18/18/18	0/3/3/3
3	FMN	G	702	-	-	0/18/18/18	0/3/3/3
3	FMN	H	1702	-	-	7/18/18/18	0/3/3/3
3	FMN	I	2702	-	-	0/18/18/18	0/3/3/3
3	FMN	B	1701	-	-	3/18/18/18	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2701	FMN	C4A-N5	4.31	1.40	1.30
3	A	701	FMN	C4A-N5	4.26	1.40	1.30
3	G	702	FMN	C4A-N5	4.19	1.39	1.30
3	E	3701	FMN	C4A-N5	4.15	1.39	1.30
3	H	1702	FMN	C4A-N5	4.10	1.39	1.30
3	B	1701	FMN	C4A-N5	4.07	1.39	1.30
3	J	3702	FMN	C4A-N5	3.74	1.38	1.30
3	I	2702	FMN	C4A-N5	3.49	1.38	1.30
3	J	3702	FMN	C10-N1	3.11	1.39	1.33
3	I	2702	FMN	C10-N1	3.03	1.39	1.33
3	D	2701	FMN	C10-N1	2.85	1.39	1.33
3	E	3701	FMN	C10-N1	2.85	1.39	1.33
3	H	1702	FMN	C10-N1	2.72	1.38	1.33
3	G	702	FMN	C10-N1	2.39	1.38	1.33
3	A	701	FMN	C10-N1	2.39	1.38	1.33
3	B	1701	FMN	C10-N1	2.32	1.37	1.33
3	J	3702	FMN	C1'-N10	2.20	1.53	1.47

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	FMN	C4-C4A-N5	3.55	123.12	118.21
3	B	1701	FMN	C4-N3-C2	-3.46	119.49	125.64
3	A	701	FMN	C4A-C10-N10	3.41	121.37	116.48
3	D	2701	FMN	C4-N3-C2	-3.41	119.59	125.64
3	B	1701	FMN	C4A-C10-N10	3.39	121.34	116.48
3	G	702	FMN	C5A-C9A-N10	3.33	120.98	117.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	702	FMN	C9A-C5A-N5	-3.31	118.94	122.45
3	G	702	FMN	C4-N3-C2	-3.28	119.81	125.64
3	A	701	FMN	O4-C4-N3	-3.27	113.97	120.11
3	H	1702	FMN	C5A-C9A-N10	3.21	120.87	117.97
3	I	2702	FMN	C4-N3-C2	-3.13	120.08	125.64
3	J	3702	FMN	C4-N3-C2	-3.12	120.10	125.64
3	A	701	FMN	C10-C4A-N5	-3.09	118.49	124.81
3	D	2701	FMN	C4A-C4-N3	3.07	121.08	113.25
3	B	1701	FMN	C10-C4A-N5	-3.05	118.58	124.81
3	E	3701	FMN	C4-C4A-N5	2.99	122.33	118.21
3	J	3702	FMN	C5A-C9A-N10	2.97	120.66	117.97
3	I	2702	FMN	O4-C4-C4A	-2.89	118.90	126.53
3	J	3702	FMN	C4A-C4-N3	2.84	120.48	113.25
3	H	1702	FMN	C4A-C10-N10	2.84	120.54	116.48
3	B	1701	FMN	C9A-C5A-N5	-2.81	119.47	122.45
3	D	2701	FMN	C4A-C10-N10	2.81	120.50	116.48
3	G	702	FMN	C4A-C10-N10	2.77	120.45	116.48
3	H	1702	FMN	C9A-C5A-N5	-2.77	119.52	122.45
3	D	2701	FMN	O5'-P-O1P	2.76	113.91	106.44
3	B	1701	FMN	C5A-C9A-N10	2.76	120.46	117.97
3	I	2702	FMN	C4A-C4-N3	2.75	120.24	113.25
3	E	3701	FMN	C4A-C10-N10	2.74	120.41	116.48
3	G	702	FMN	C10-C4A-N5	-2.72	119.26	124.81
3	E	3701	FMN	C10-C4A-N5	-2.66	119.37	124.81
3	E	3701	FMN	C9A-C5A-N5	-2.59	119.70	122.45
3	B	1701	FMN	C4A-C4-N3	2.59	119.83	113.25
3	H	1702	FMN	C4A-C4-N3	2.55	119.75	113.25
3	D	2701	FMN	C5A-C9A-N10	2.54	120.27	117.97
3	H	1702	FMN	C4-N3-C2	-2.52	121.16	125.64
3	J	3702	FMN	C9A-C5A-N5	-2.51	119.79	122.45
3	D	2701	FMN	C10-C4A-N5	-2.48	119.75	124.81
3	B	1701	FMN	C4-C4A-N5	2.47	121.62	118.21
3	G	702	FMN	O2P-P-O5'	2.46	113.09	106.67
3	E	3701	FMN	C4A-C4-N3	2.46	119.51	113.25
3	H	1702	FMN	C10-C4A-N5	-2.41	119.88	124.81
3	I	2702	FMN	C10-C4A-N5	-2.40	119.91	124.81
3	E	3701	FMN	C4-N3-C2	-2.39	121.39	125.64
3	J	3702	FMN	O4-C4-C4A	-2.37	120.28	126.53
3	D	2701	FMN	C4-C4A-N5	2.37	121.48	118.21
3	H	1702	FMN	C4-C4A-N5	2.36	121.46	118.21
3	J	3702	FMN	C4A-C10-N10	2.32	119.80	116.48
3	G	702	FMN	C4A-C4-N3	2.31	119.12	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2701	FMN	C9A-C5A-N5	-2.28	120.04	122.45
3	B	1701	FMN	C10-N1-C2	2.21	121.64	116.85
3	B	1701	FMN	C4A-C10-N1	-2.21	119.17	124.59
3	J	3702	FMN	C4A-C10-N1	-2.18	119.24	124.59
3	I	2702	FMN	C4A-C10-N10	2.16	119.58	116.48
3	B	1701	FMN	O2-C2-N1	-2.15	118.23	121.80
3	A	701	FMN	C4A-C4-N3	2.14	118.70	113.25
3	G	702	FMN	O4-C4-C4A	-2.13	120.90	126.53
3	B	1701	FMN	O4-C4-C4A	-2.11	120.95	126.53
3	D	2701	FMN	C4A-C10-N1	-2.11	119.42	124.59
3	B	1701	FMN	C8M-C8-C9	-2.11	115.86	119.57
3	A	701	FMN	C5'-C4'-C3'	2.09	116.17	112.22
3	I	2702	FMN	C9A-C5A-N5	-2.09	120.24	122.45
3	A	701	FMN	O2P-P-O5'	2.06	112.03	106.67
3	E	3701	FMN	C5A-C9A-N10	2.05	119.82	117.97
3	B	1701	FMN	C7M-C7-C6	-2.03	116.00	119.57

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	FMN	C5'-O5'-P-O1P
3	B	1701	FMN	C5'-O5'-P-O1P
3	B	1701	FMN	C5'-O5'-P-O2P
3	H	1702	FMN	C5'-O5'-P-O2P
3	J	3702	FMN	C5'-O5'-P-O1P
3	J	3702	FMN	C5'-O5'-P-O2P
3	H	1702	FMN	O2'-C2'-C3'-C4'
3	E	3701	FMN	C2'-C3'-C4'-C5'
3	E	3701	FMN	C2'-C3'-C4'-O4'
3	D	2701	FMN	C5'-O5'-P-O1P
3	H	1702	FMN	C5'-O5'-P-O1P
3	E	3701	FMN	O3'-C3'-C4'-C5'
3	E	3701	FMN	O3'-C3'-C4'-O4'
3	H	1702	FMN	O2'-C2'-C3'-O3'
3	H	1702	FMN	C1'-C2'-C3'-O3'
3	E	3701	FMN	C5'-O5'-P-O1P
3	D	2701	FMN	C2'-C3'-C4'-C5'
3	A	701	FMN	C5'-O5'-P-O2P
3	B	1701	FMN	C5'-O5'-P-O3P
3	D	2701	FMN	C5'-O5'-P-O2P
3	H	1702	FMN	C5'-O5'-P-O3P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	J	3702	FMN	C5'-O5'-P-O3P
3	H	1702	FMN	C2'-C3'-C4'-O4'

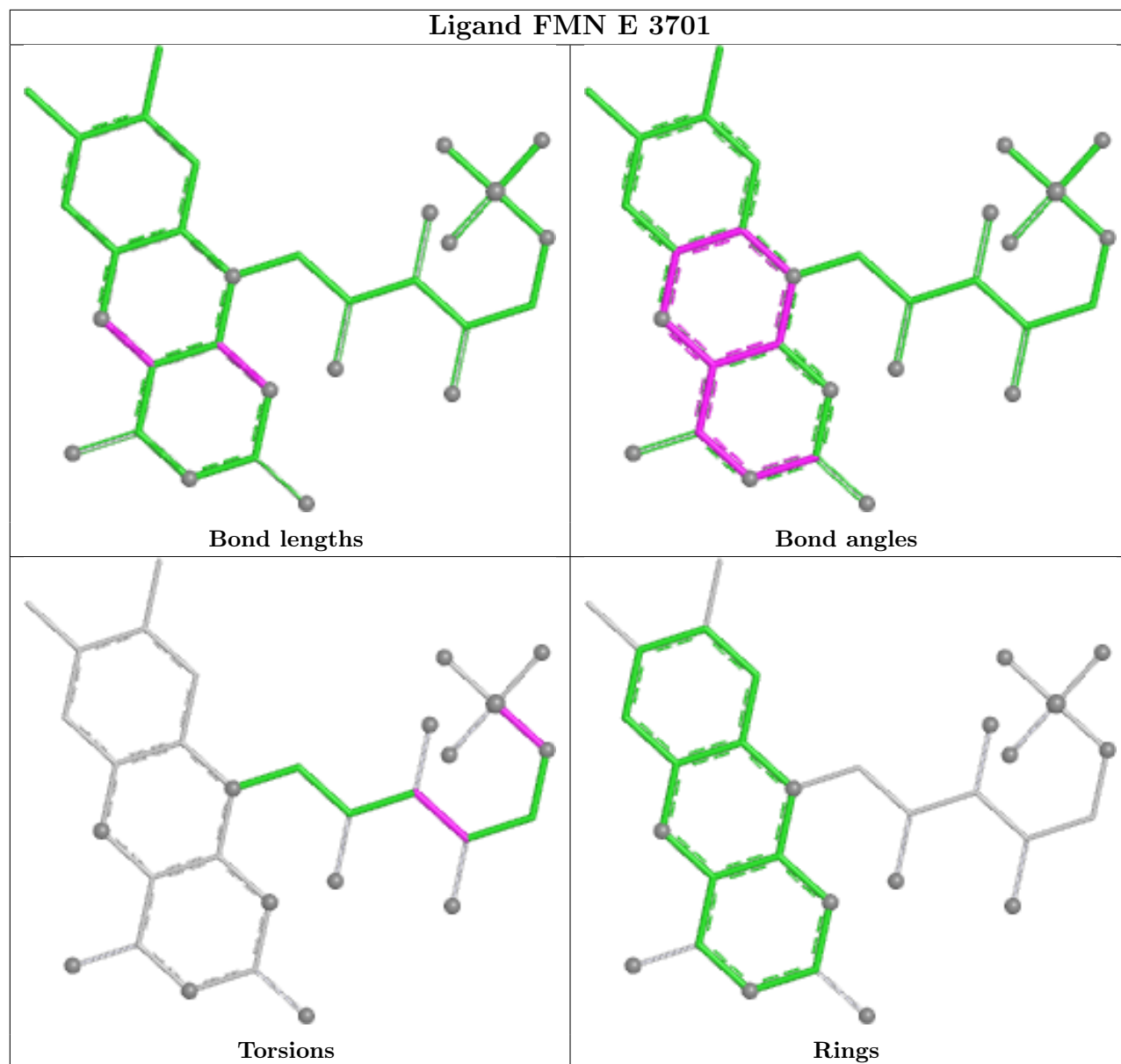
There are no ring outliers.

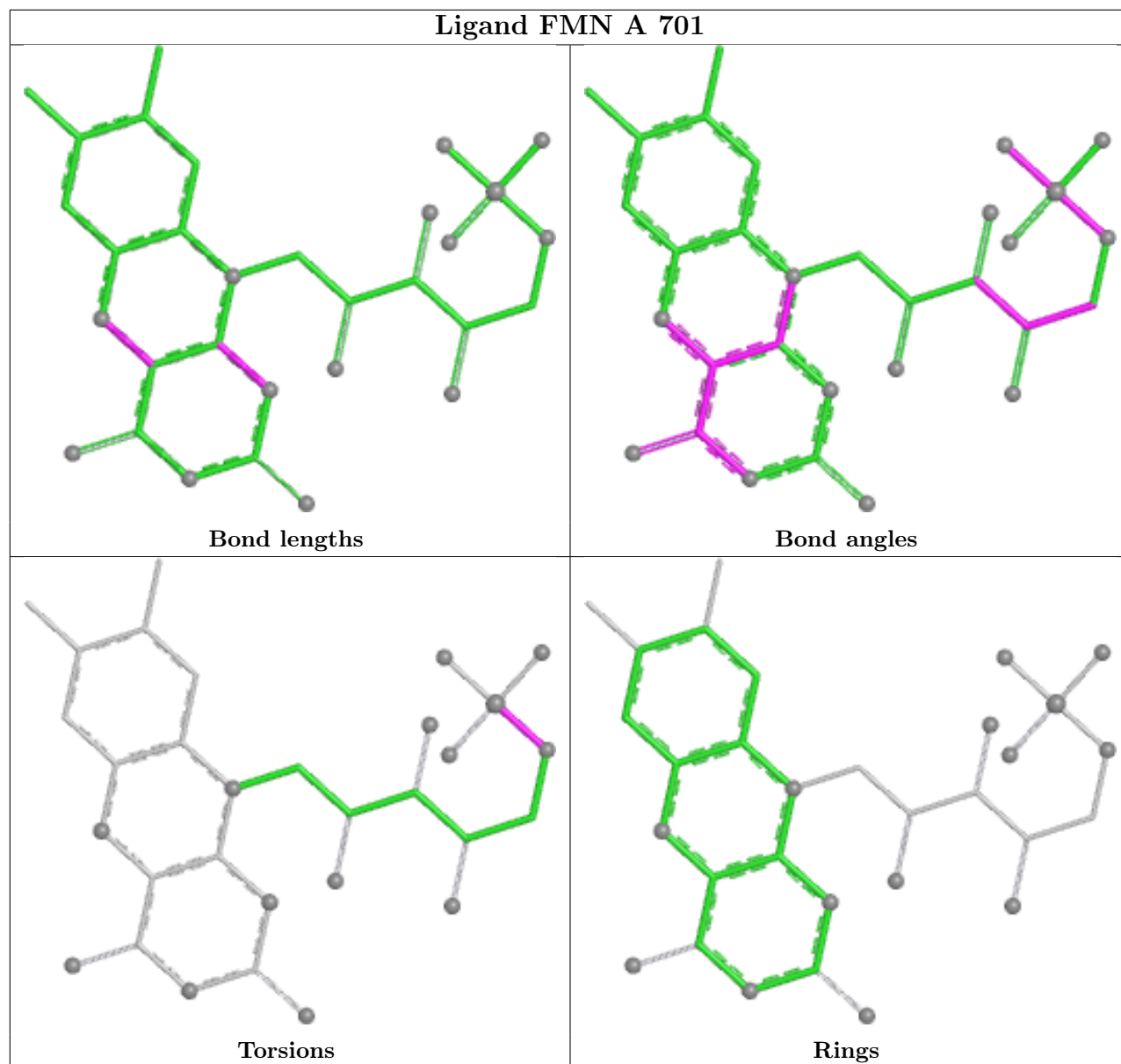
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	2702	FMN	1	0

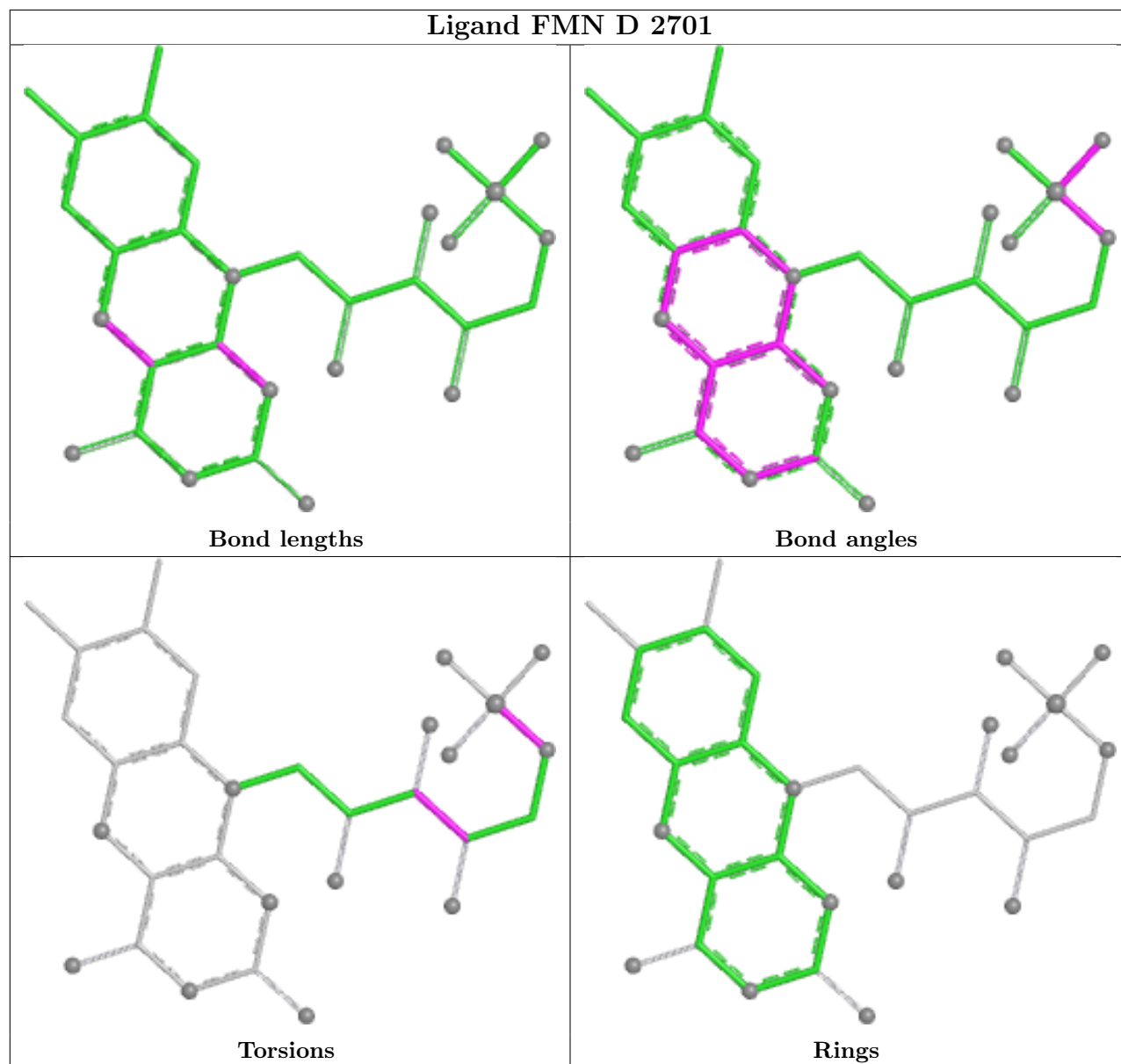
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand FMN E 3701

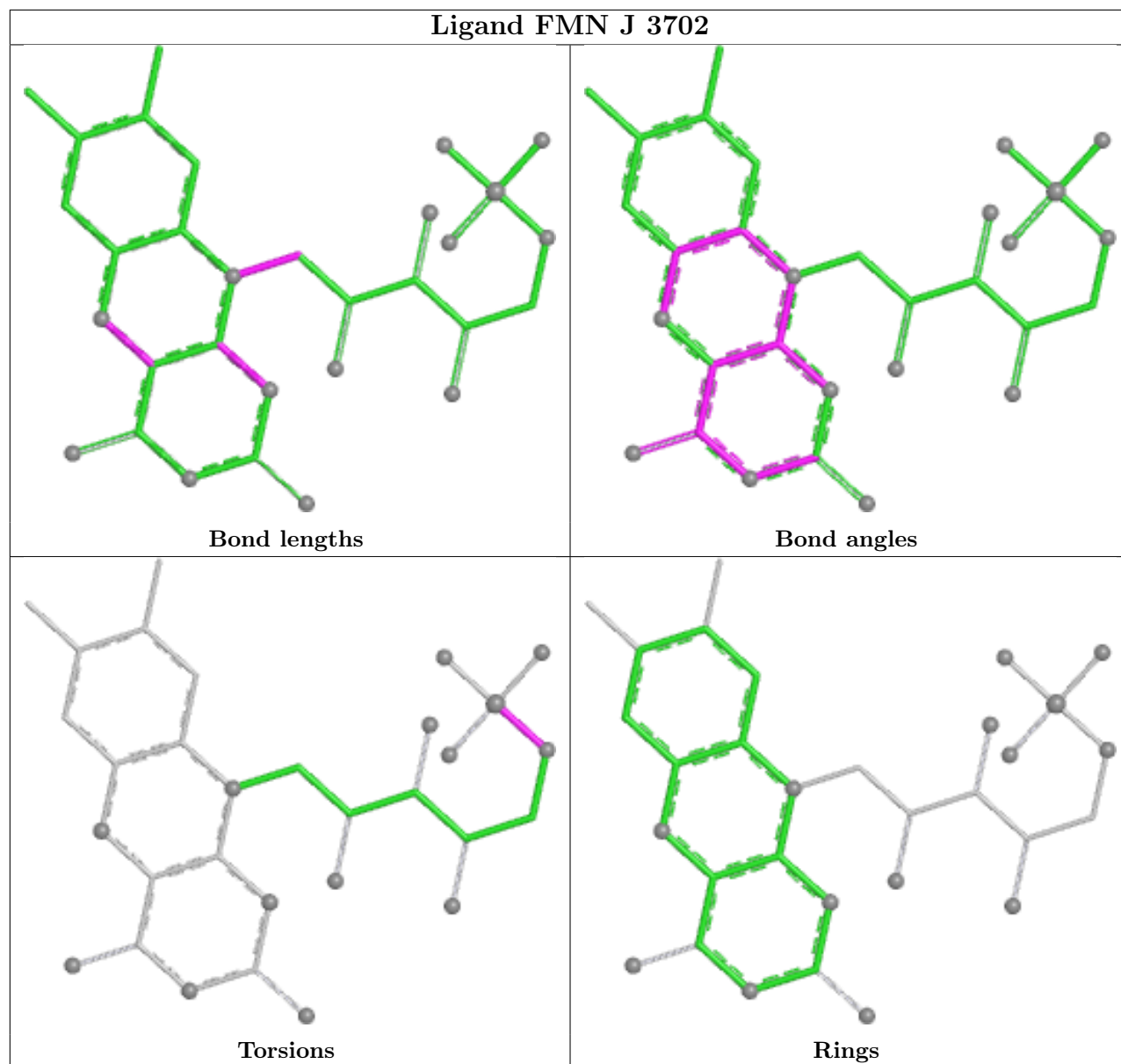


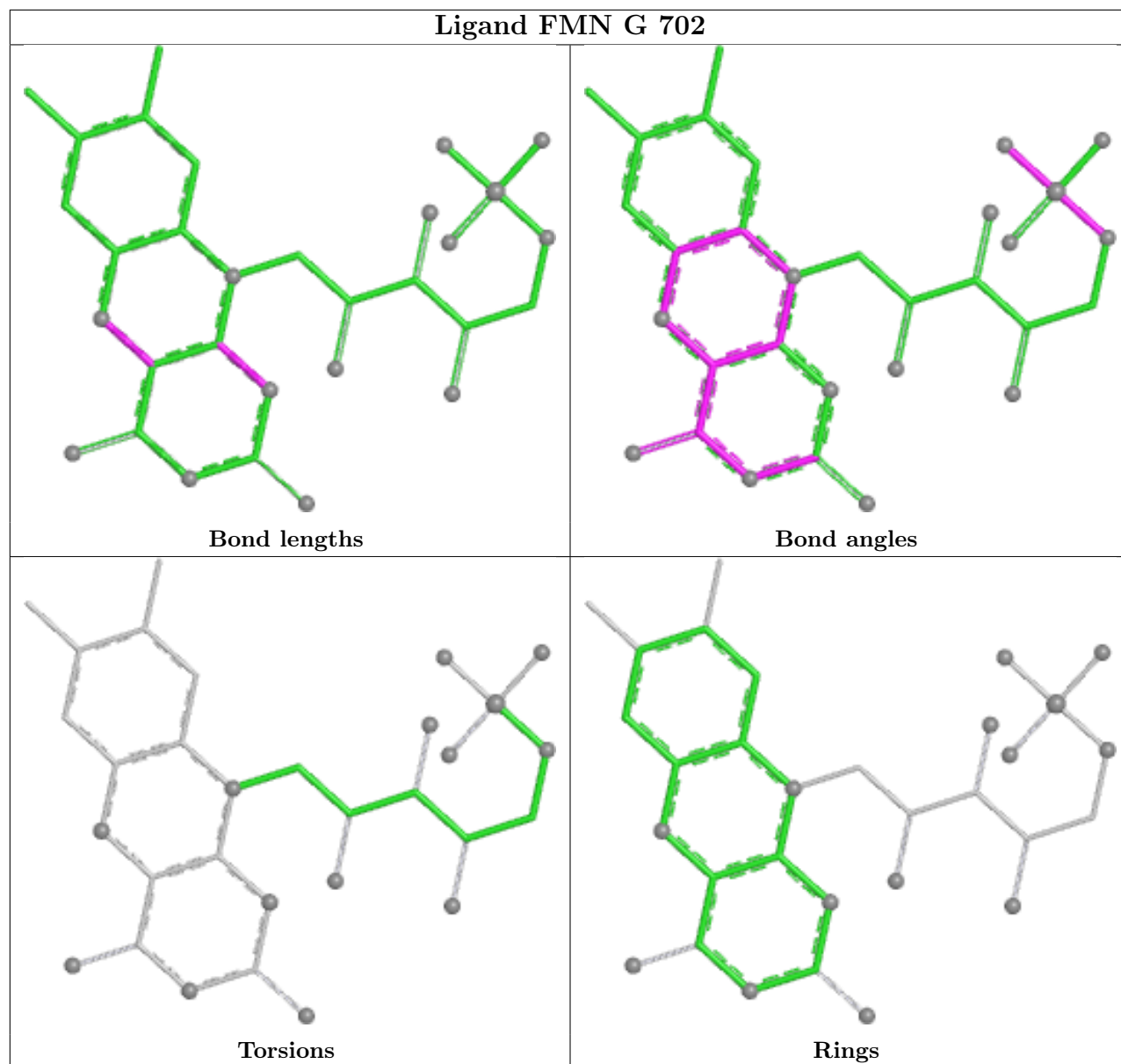


Ligand FMN D 2701

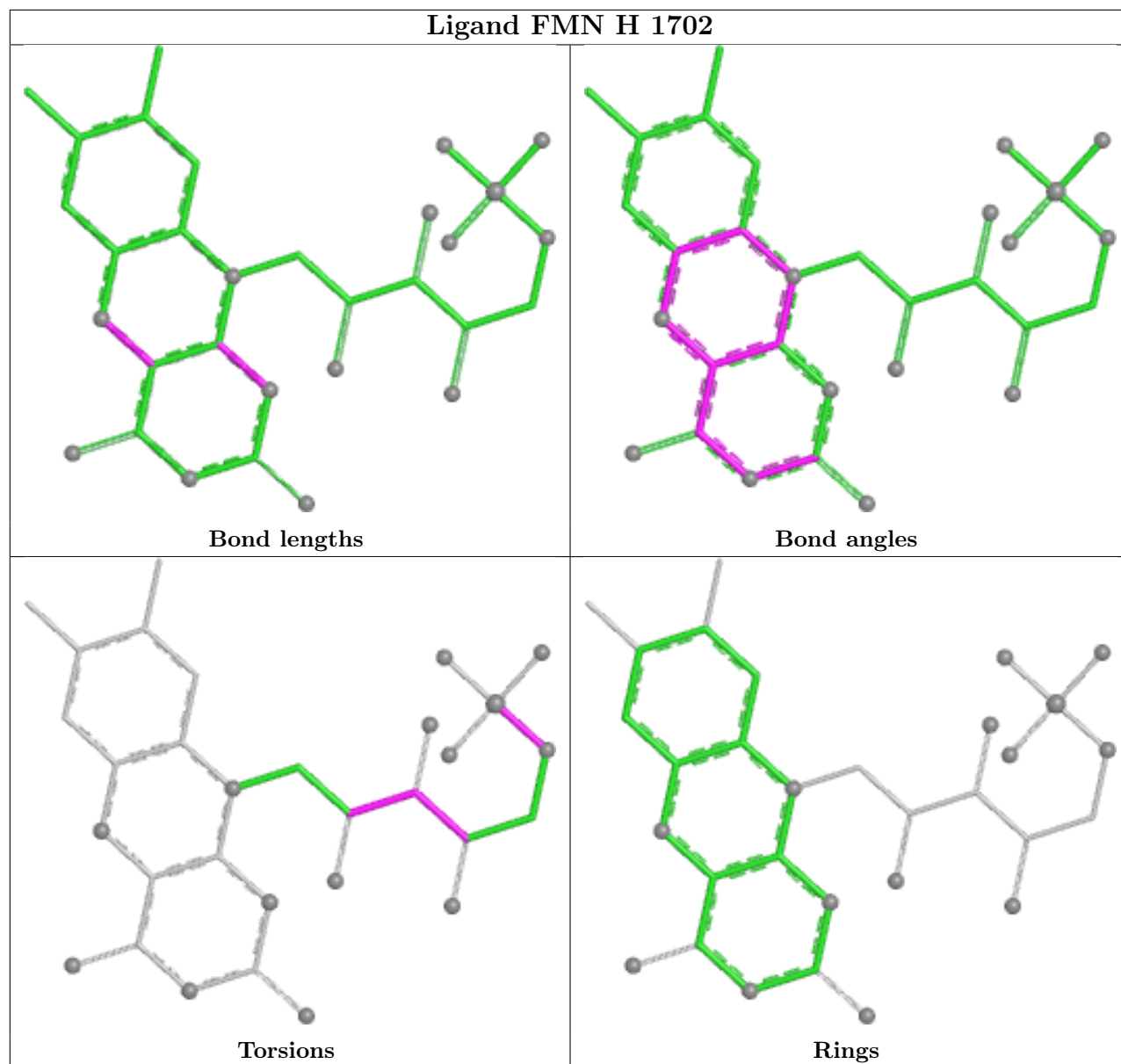


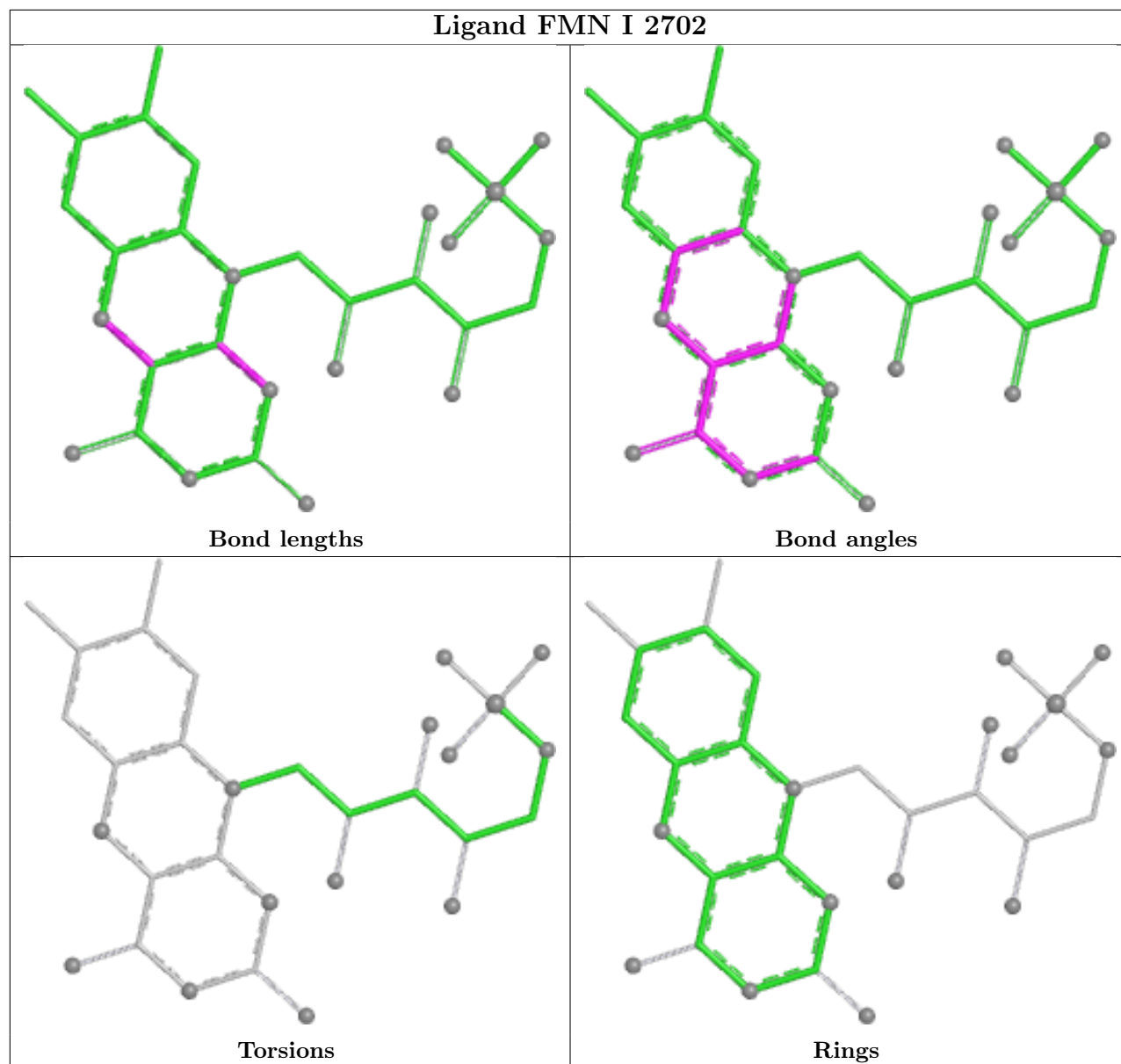
Ligand FMN J 3702

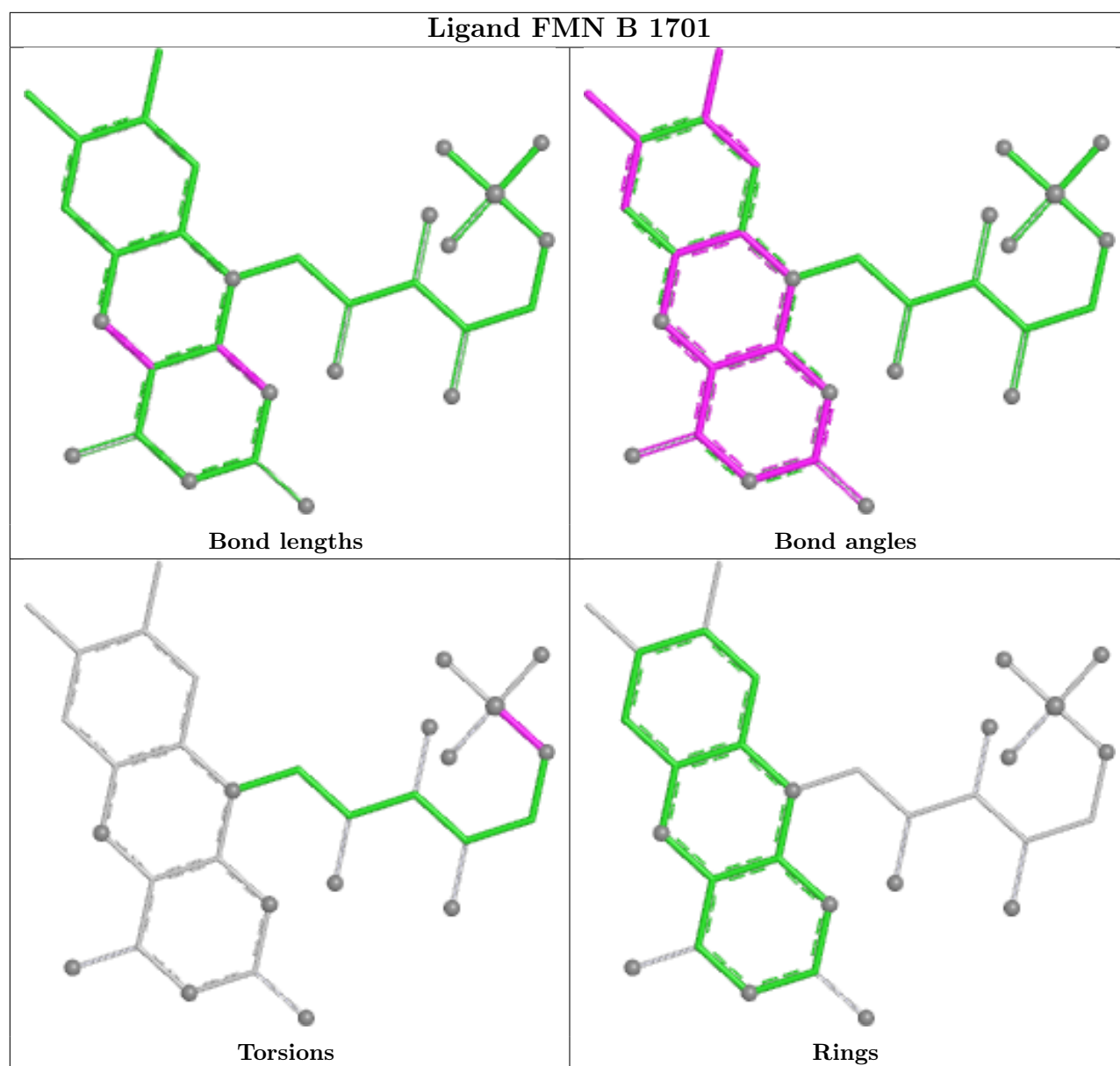




Ligand FMN H 1702







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	403/404 (99%)	0.65	15 (3%)	45	48	29, 43, 56, 64	1 (0%)
1	B	403/404 (99%)	0.45	7 (1%)	69	70	35, 43, 56, 65	0
1	D	403/404 (99%)	0.38	8 (1%)	65	66	30, 42, 55, 64	3 (0%)
1	E	403/404 (99%)	0.78	18 (4%)	38	40	35, 43, 55, 64	1 (0%)
1	G	403/404 (99%)	0.49	12 (2%)	52	54	30, 42, 55, 65	1 (0%)
1	H	403/404 (99%)	0.67	27 (6%)	24	26	35, 43, 55, 65	0
1	I	403/404 (99%)	0.63	15 (3%)	45	48	35, 43, 55, 63	0
1	J	403/404 (99%)	0.35	13 (3%)	50	52	31, 42, 56, 65	2 (0%)
All	All	3224/3232 (99%)	0.55	115 (3%)	46	48	29, 43, 56, 65	8 (0%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	221	GLY	5.3
1	J	375	CYS	4.4
1	H	360	GLY	3.9
1	H	217	VAL	3.8
1	I	226	ILE	3.8
1	E	152	TRP	3.6
1	H	297	ASP	3.6
1	E	226	ILE	3.6
1	G	221	GLY	3.5
1	I	223	LEU	3.5
1	J	152	TRP	3.4
1	E	194	ALA	3.1
1	H	250	TRP	3.1
1	D	152	TRP	3.1
1	E	246	ALA	3.0
1	I	369	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	221	GLY	3.0
1	G	44	GLU	2.9
1	A	152	TRP	2.9
1	E	128	THR	2.9
1	A	374	ALA	2.9
1	D	375	CYS	2.9
1	I	154	ASP	2.9
1	G	27	GLY	2.8
1	E	110	ALA	2.8
1	D	225	ARG	2.8
1	E	42	GLY	2.8
1	B	149	LEU	2.8
1	G	123	GLU	2.8
1	G	77	ASP	2.8
1	H	32	GLY	2.8
1	G	43	ASP	2.7
1	G	374	ALA	2.7
1	I	217	VAL	2.7
1	I	152	TRP	2.7
1	H	149	LEU	2.7
1	H	194	ALA	2.6
1	A	223	LEU	2.6
1	H	152	TRP	2.6
1	J	368	GLU	2.6
1	E	240	PRO	2.6
1	E	150	LEU	2.6
1	J	299	SER	2.6
1	H	127	MET	2.6
1	A	249	GLY	2.5
1	H	249	GLY	2.5
1	J	151	HIS	2.5
1	A	224	GLU	2.5
1	B	152	TRP	2.5
1	H	87	ASP	2.5
1	E	129	VAL	2.5
1	B	150	LEU	2.5
1	G	375	CYS	2.4
1	I	128	THR	2.4
1	D	150	LEU	2.4
1	I	149	LEU	2.4
1	I	163	ASP	2.4
1	E	225	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	42	GLY	2.4
1	H	225	ARG	2.4
1	E	29	THR	2.4
1	H	243	ILE	2.4
1	E	250	TRP	2.4
1	D	353	GLY	2.4
1	I	251	ALA	2.4
1	H	189	TYR	2.4
1	B	123	GLU	2.4
1	J	169	ASN	2.4
1	B	27	GLY	2.4
1	G	120	SER	2.4
1	H	155	SER	2.4
1	I	151	HIS	2.4
1	B	374	ALA	2.3
1	A	162	GLU	2.3
1	H	62	ALA	2.3
1	J	26	HIS	2.3
1	H	205	PRO	2.3
1	A	45	GLY	2.3
1	E	141	THR	2.3
1	E	223	LEU	2.2
1	E	177	CYS	2.2
1	A	83	HIS	2.2
1	A	195	ALA	2.2
1	H	374	ALA	2.2
1	G	147	THR	2.2
1	J	294	HIS	2.2
1	A	115	LEU	2.2
1	J	364	GLU	2.2
1	A	70	GLN	2.2
1	I	372	ASP	2.2
1	H	240	PRO	2.2
1	A	42	GLY	2.2
1	A	206	LEU	2.2
1	E	20	TRP	2.1
1	H	220	LEU	2.1
1	J	87	ASP	2.1
1	J	255	VAL	2.1
1	G	41	CYS	2.1
1	D	149	LEU	2.1
1	D	223	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	282	MET	2.1
1	I	78	TYR	2.1
1	B	215	ASP	2.1
1	A	317	THR	2.1
1	H	25	TYR	2.1
1	G	152	TRP	2.1
1	A	72	GLY	2.1
1	D	280	GLY	2.1
1	H	29	THR	2.1
1	H	246	ALA	2.1
1	J	225	ARG	2.1
1	H	351	SER	2.0
1	H	90	GLY	2.0
1	H	24	ASN	2.0
1	I	50	ASP	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($\text{\AA}^2$)	Q<0.9
4	CL	J	3505	1/1	0.82	0.10	37,37,37,37	1
2	FE	I	2503	1/1	0.85	0.10	63,63,63,63	1
2	FE	E	3503	1/1	0.85	0.10	58,58,58,58	1
4	CL	H	1504	1/1	0.87	0.12	47,47,47,47	1
3	FMN	D	2701	31/31	0.88	0.11	37,40,43,44	0
3	FMN	B	1701	31/31	0.90	0.10	33,35,39,40	0
2	FE	D	2503	1/1	0.91	0.11	36,36,36,36	1
4	CL	J	3504	1/1	0.91	0.10	36,36,36,36	1

Continued on next page...

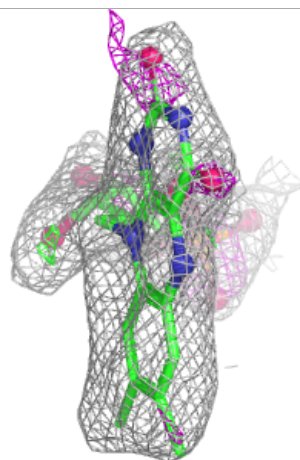
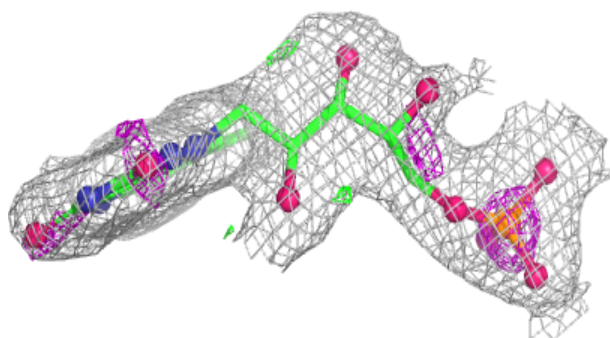
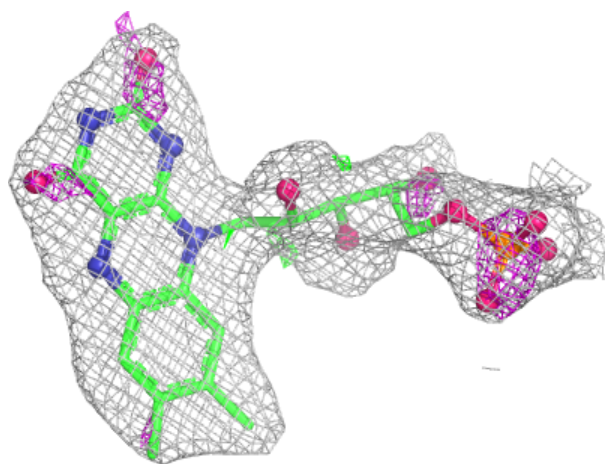
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FMN	G	702	31/31	0.91	0.10	29,32,34,35	0
3	FMN	J	3702	31/31	0.92	0.09	38,41,42,42	0
3	FMN	I	2702	31/31	0.92	0.09	29,33,34,35	0
4	CL	D	2504	1/1	0.93	0.17	41,41,41,41	1
2	FE	H	1503	1/1	0.93	0.14	44,44,44,44	1
2	FE	B	1503	1/1	0.93	0.15	45,45,45,45	1
3	FMN	E	3701	31/31	0.93	0.09	29,32,33,34	0
2	FE	J	3503	1/1	0.94	0.10	48,48,48,48	1
3	FMN	H	1702	31/31	0.94	0.09	28,35,36,36	0
3	FMN	A	701	31/31	0.95	0.08	24,33,34,35	0
2	FE	E	3501	1/1	0.97	0.13	44,44,44,44	0
2	FE	A	503	1/1	0.97	0.18	47,47,47,47	1
2	FE	H	1501	1/1	0.97	0.09	47,47,47,47	0
2	FE	G	503	1/1	0.98	0.09	32,32,32,32	1
2	FE	B	1501	1/1	0.98	0.09	36,36,36,36	0
2	FE	A	501	1/1	0.98	0.12	45,45,45,45	0
2	FE	I	2501	1/1	0.98	0.09	48,48,48,48	0
2	FE	D	2501	1/1	0.98	0.09	39,39,39,39	0
2	FE	G	501	1/1	0.98	0.10	37,37,37,37	0
2	FE	J	3501	1/1	0.99	0.08	37,37,37,37	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.

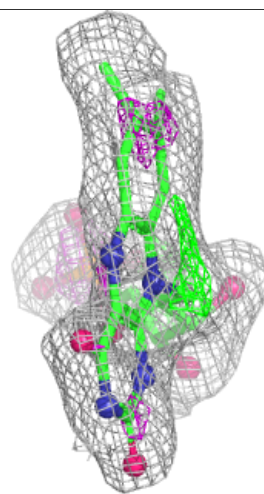
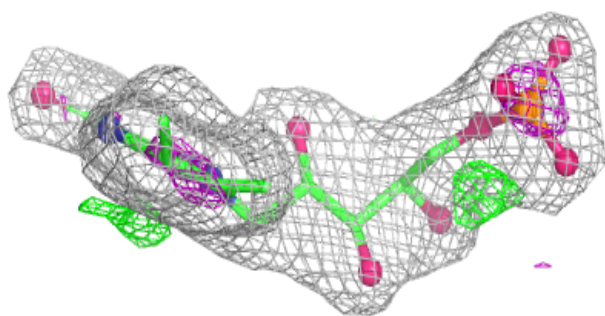
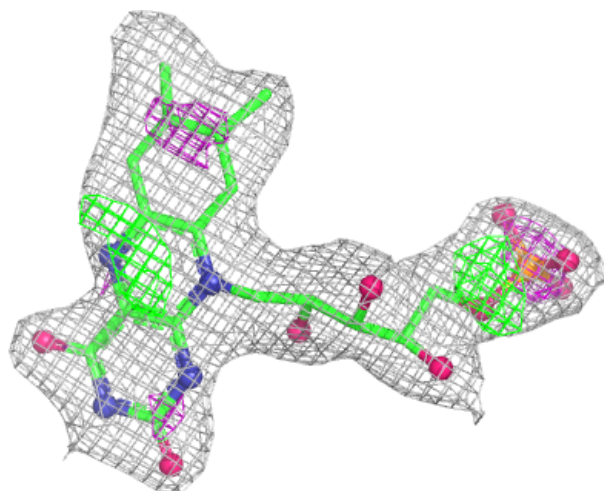
Electron density around FMN D 2701:

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



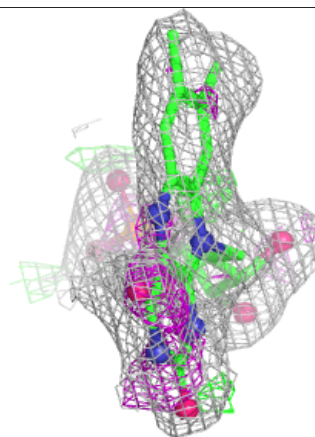
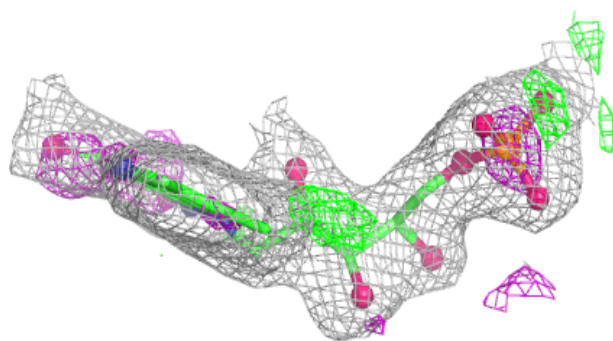
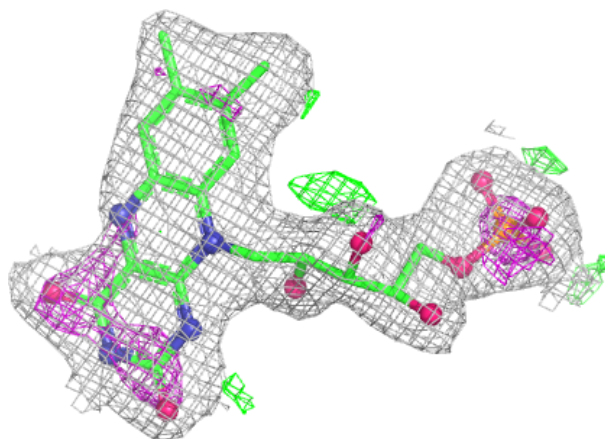
Electron density around FMN B 1701:

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



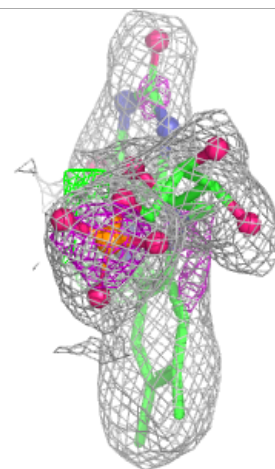
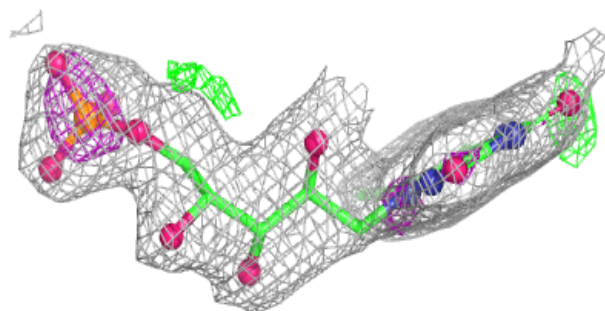
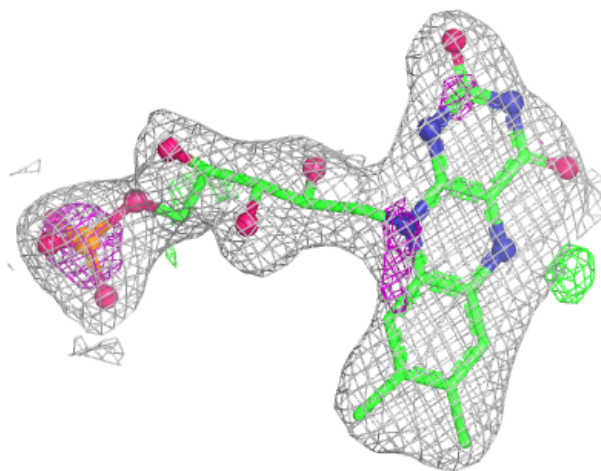
Electron density around FMN G 702:

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



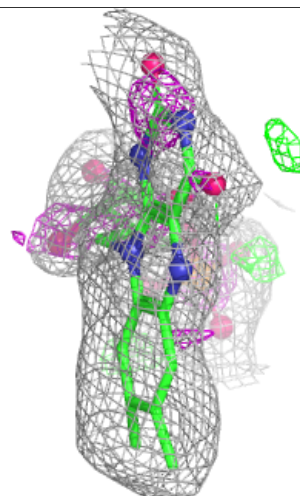
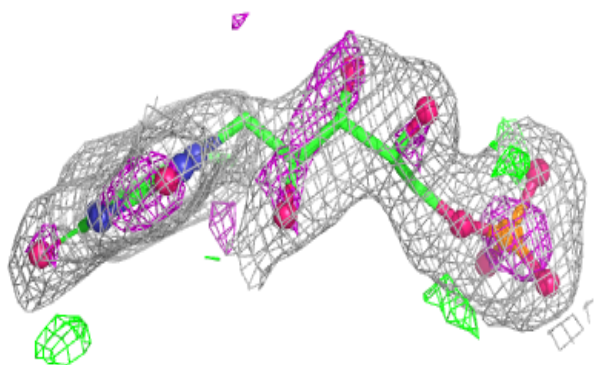
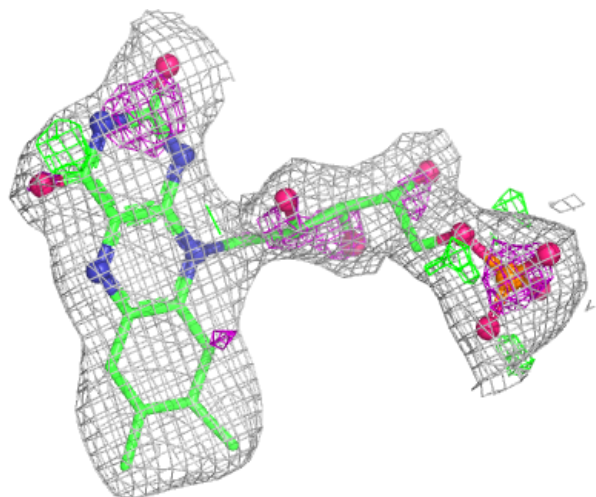
Electron density around FMN J 3702:

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



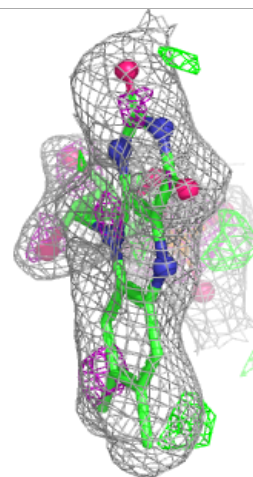
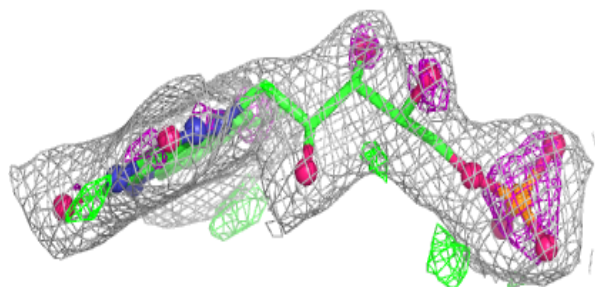
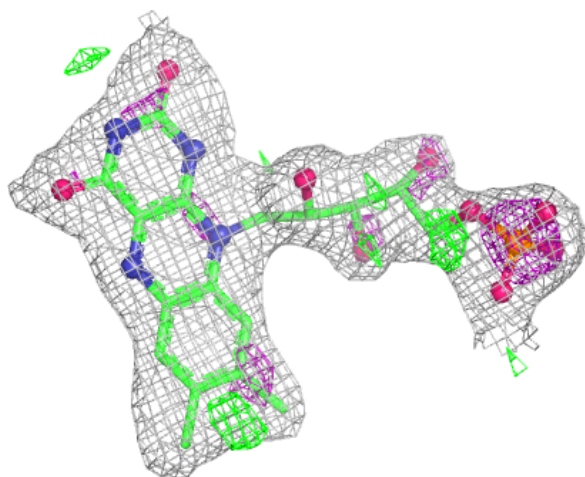
Electron density around FMN I 2702:

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



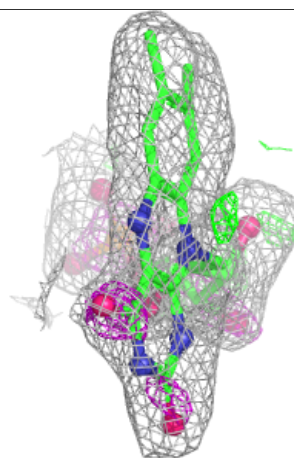
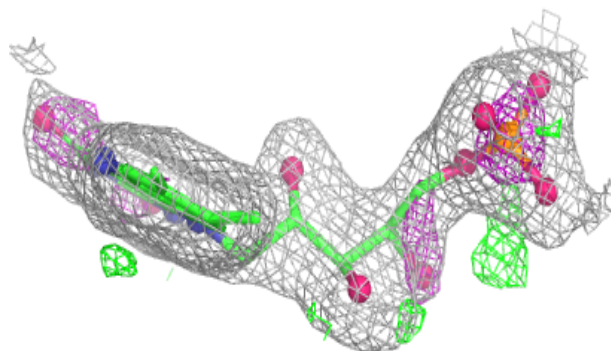
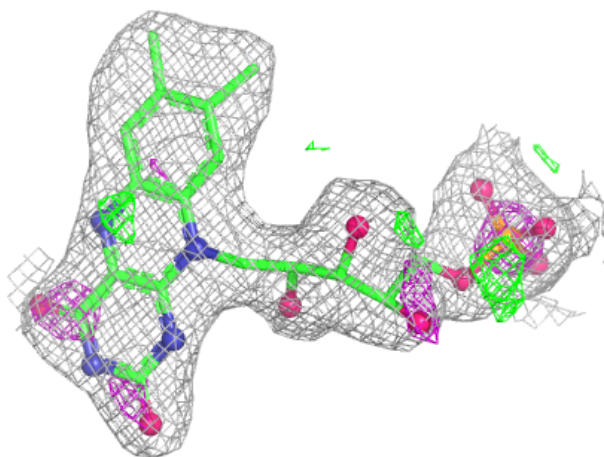
Electron density around FMN E 3701:

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



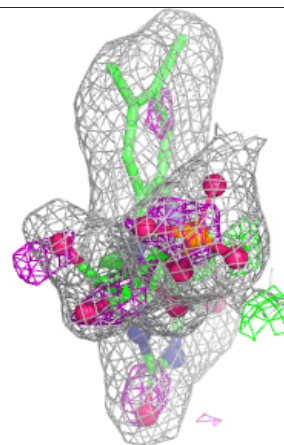
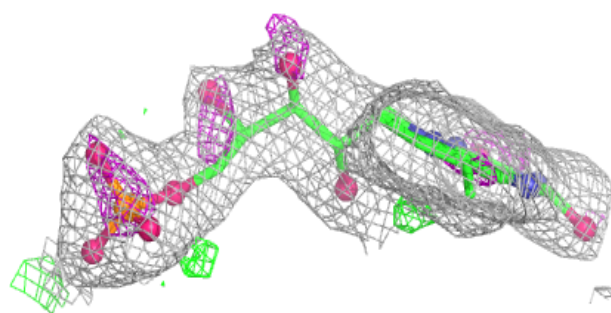
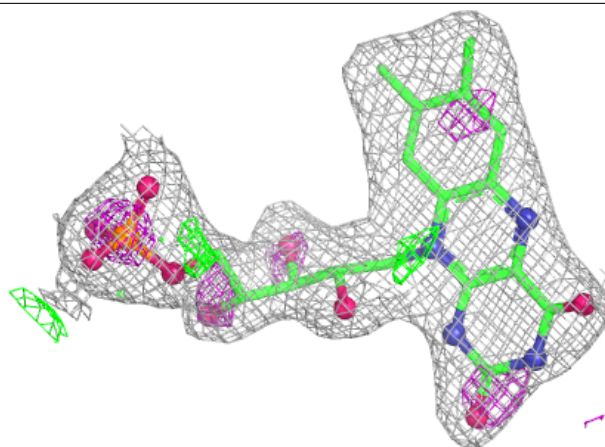
Electron density around FMN H 1702:

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



Electron density around FMN A 701:

$2mF_o - DF_c$ (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.