



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:56 PM UTC

PDB ID : 3F6S / pdb_00003f6s
Title : Desulfovibrio desulfuricans (ATCC 29577) oxidized flavodoxin alternate conformers
Authors : Guelker, M.; Shamoo, Y.
Deposited on : 2008-11-06
Resolution : 2.50 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

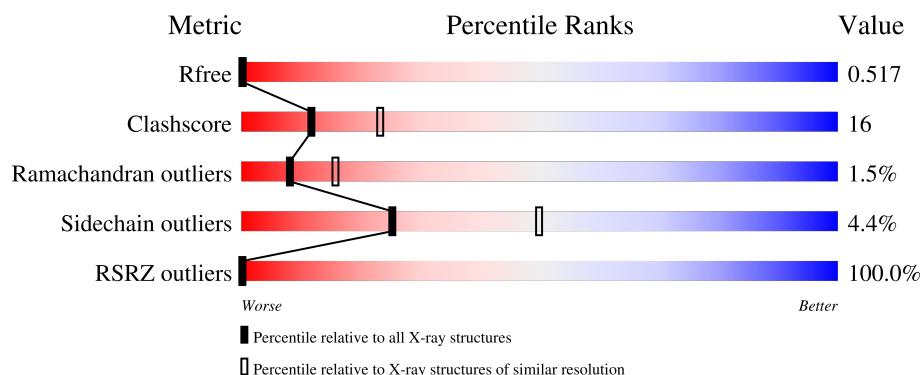
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	148	99% 76% 18% 5% ..
1	B	148	99% 76% 19% ..
1	D	148	99% 69% 29% ..
1	E	148	99% 68% 28% ..
1	F	148	99% 66% 32% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	148	99% 76%19% ..
1	H	148	99% 63%34% ..
1	I	148	99% 72%26% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FMN	D	151	-	-	-	X
2	FMN	E	152	-	-	-	X
2	FMN	F	153	-	-	-	X
2	FMN	H	154	-	-	-	X
2	FMN	I	155	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9299 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.

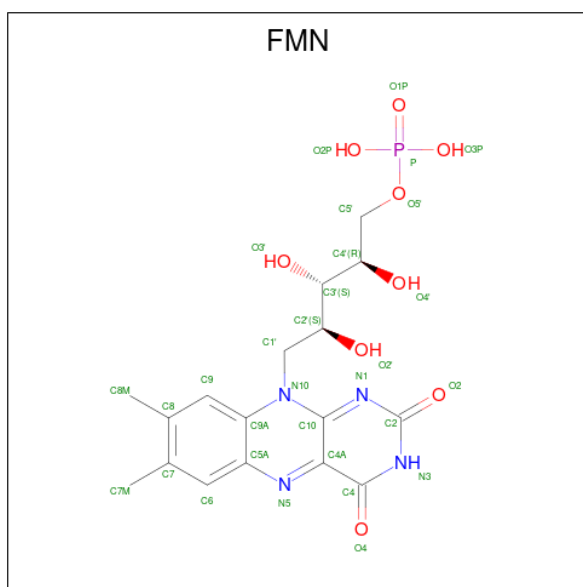
- Molecule 1 is a protein called Flavodoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	0	0
			1093	683	175	230	5			
1	B	147	Total	C	N	O	S	0	0	0
			1093	683	175	230	5			
1	D	147	Total	C	N	O	S	0	0	0
			1093	683	175	230	5			
1	E	147	Total	C	N	O	S	0	0	0
			1093	683	175	230	5			
1	F	147	Total	C	N	O	S	0	0	0
			1093	683	175	230	5			
1	H	147	Total	C	N	O	S	0	0	0
			1093	683	175	230	5			
1	I	147	Total	C	N	O	S	0	0	0
			1093	683	175	230	5			
1	G	147	Total	C	N	O	S	0	0	0
			1093	683	175	230	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	ASP	ASN	engineered mutation	UNP P26492
B	79	ASP	ASN	engineered mutation	UNP P26492
D	79	ASP	ASN	engineered mutation	UNP P26492
E	79	ASP	ASN	engineered mutation	UNP P26492
F	79	ASP	ASN	engineered mutation	UNP P26492
H	79	ASP	ASN	engineered mutation	UNP P26492
I	79	ASP	ASN	engineered mutation	UNP P26492
G	79	ASP	ASN	engineered mutation	UNP P26492

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	68	Total	O	0	0
			68	68		
3	D	17	Total	O	0	0
			17	17		
3	E	43	Total	O	0	0
			43	43		

Continued on next page...

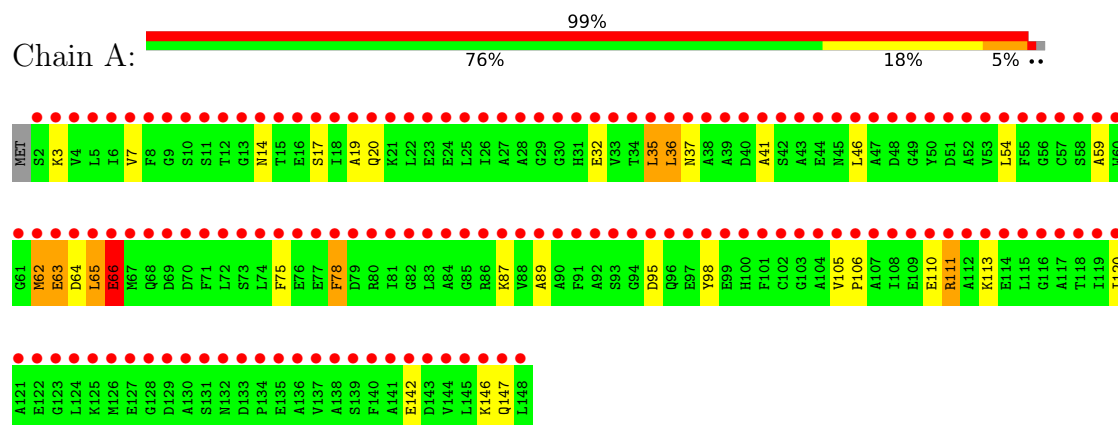
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	26	Total 26	O 26	0	0
3	H	34	Total 34	O 34	0	0
3	I	32	Total 32	O 32	0	0
3	G	40	Total 40	O 40	0	0

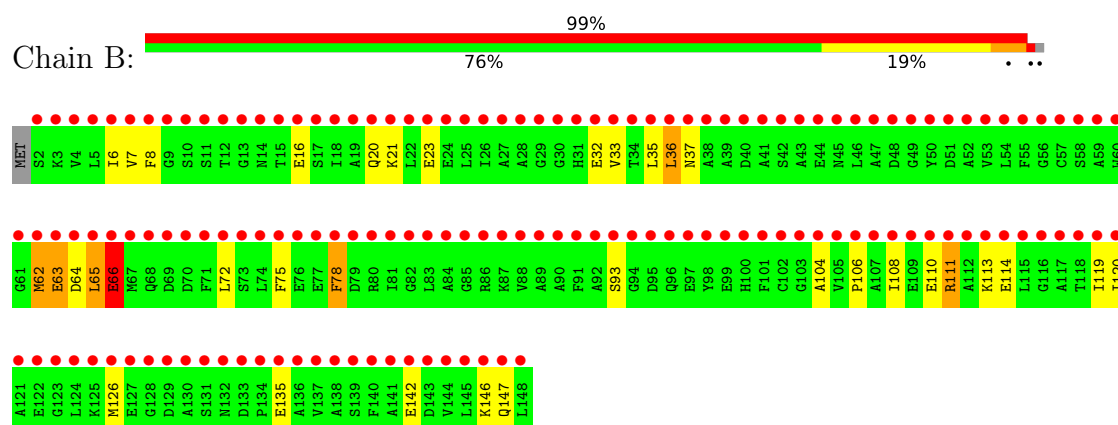
3 Residue-property plots

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

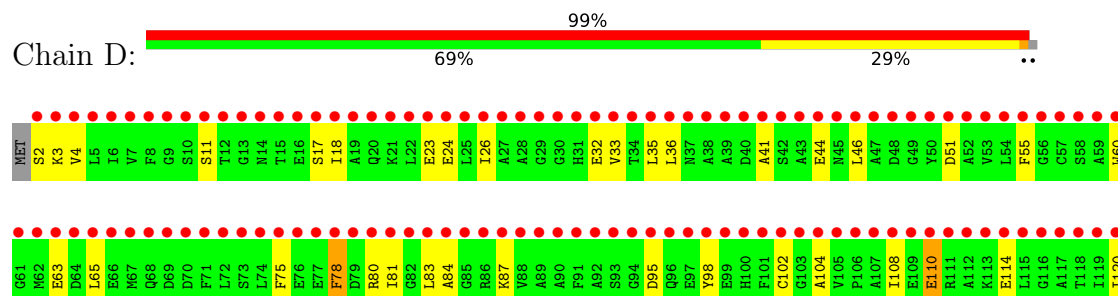
• Molecule 1: Flavodoxin

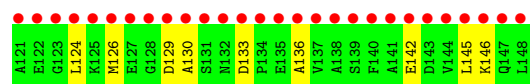


• Molecule 1: Flavodoxin

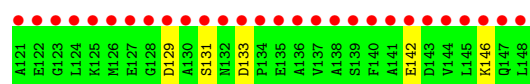
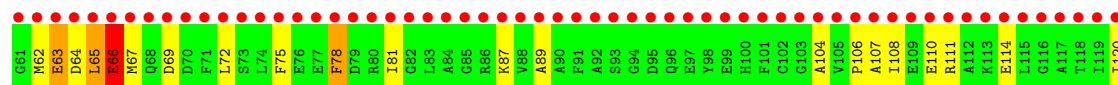
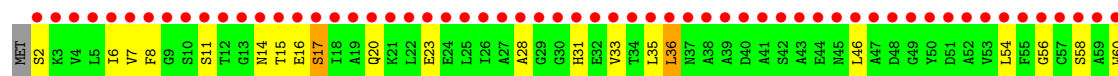


• Molecule 1: Flavodoxin

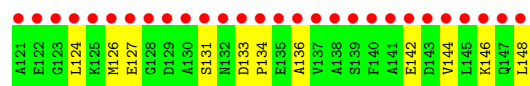
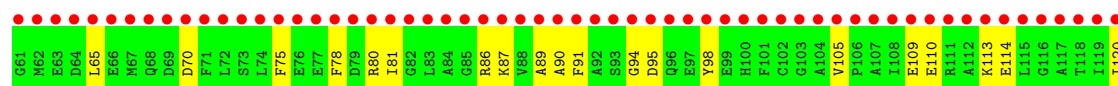
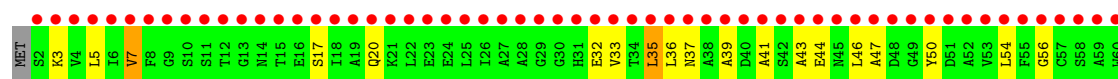




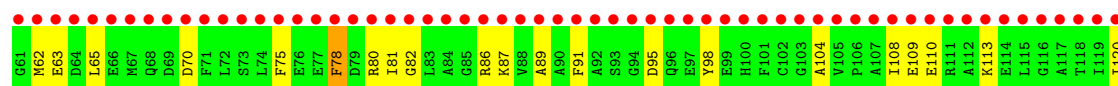
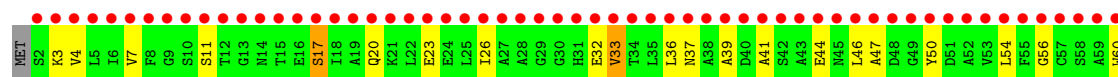
• Molecule 1: Flavodoxin



• Molecule 1: Flavodoxin

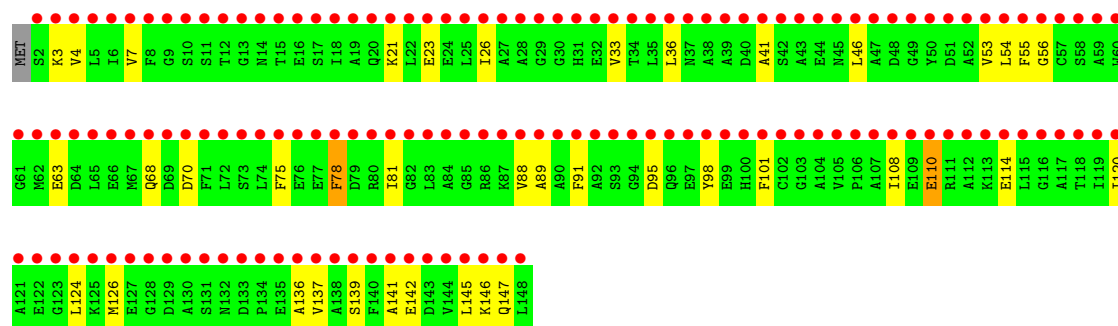


• Molecule 1: Flavodoxin

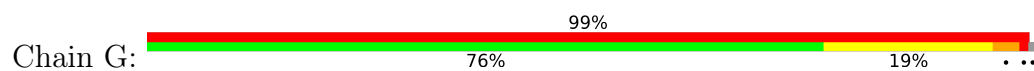


• Molecule 1: Flavodoxin





● Molecule 1: Flavodoxin



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	94.89Å 94.89Å 238.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.89 – 2.50 19.89 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.89-2.50) 99.6 (19.89-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.10 (at 2.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine), CNS	Depositor
R, R_{free}	0.220 , 0.279 0.517 , 0.517	Depositor DCC
R_{free} test set	4386 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å ²)	10.6	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 100.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.053 for -h,-k,l	Xtriage
Reported twinning fraction	0.071 for H, K, L 0.929 for -h,-k,l	Depositor
Outliers	13 of 43606 reflections (0.030%)	Xtriage
F_o, F_c correlation	0.50	EDS
Total number of atoms	9299	wwPDB-VP
Average B, all atoms (Å ²)	67.0	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 70.32 % 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 3.1875e-06. 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: FMN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.47	0/1108	0.81	1/1494 (0.1%)
1	B	0.48	0/1108	0.83	1/1494 (0.1%)
1	D	0.37	0/1108	0.70	0/1494
1	E	0.49	0/1108	0.87	3/1494 (0.2%)
1	F	0.38	0/1108	0.72	2/1494 (0.1%)
1	G	0.47	0/1108	0.83	1/1494 (0.1%)
1	H	0.39	0/1108	0.72	2/1494 (0.1%)
1	I	0.37	0/1108	0.75	0/1494
All	All	0.43	0/8864	0.78	10/11952 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	66	GLU	N-CA-C	6.21	124.03	110.80
1	G	66	GLU	N-CA-C	5.76	123.07	110.80
1	A	66	GLU	N-CA-C	5.74	123.03	110.80
1	B	66	GLU	N-CA-C	5.72	122.99	110.80
1	E	133	ASP	CA-C-N	5.63	125.30	119.05
1	E	133	ASP	C-N-CA	5.63	125.30	119.05
1	F	133	ASP	CA-C-N	5.60	125.44	119.28
1	F	133	ASP	C-N-CA	5.60	125.44	119.28
1	H	133	ASP	CA-C-N	5.42	125.08	119.56
1	H	133	ASP	C-N-CA	5.42	125.08	119.56

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	A	1093	0	1038	32	0
1	B	1093	0	1038	30	0
1	D	1093	0	1038	34	0
1	E	1093	0	1038	39	0
1	F	1093	0	1038	42	0
1	G	1093	0	1038	28	0
1	H	1093	0	1038	46	0
1	I	1093	0	1038	33	0
2	A	31	0	19	3	0
2	B	31	0	19	0	0
2	D	31	0	19	1	0
2	E	31	0	19	2	0
2	F	31	0	19	0	0
2	G	31	0	19	0	0
2	H	31	0	19	0	0
2	I	31	0	19	1	0
3	A	47	0	0	2	0
3	B	68	0	0	2	0
3	D	17	0	0	0	0
3	E	43	0	0	1	0
3	F	26	0	0	0	0
3	G	40	0	0	2	0
3	H	34	0	0	0	0
3	I	32	0	0	0	0
All	All	9299	0	8456	277	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 16.

All (277) 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:I:124:LEU:HD11	1:I:126:MET:HE3	1.42	1.02
1:D:4:VAL:HB	1:D:33:VAL:HG12	1.49	0.93
1:E:142:GLU:HG2	1:E:146:LYS:HE3	1.52	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:124:LEU:HD21	1:H:126:MET:HE3	1.51	0.91
1:F:95:ASP:HB3	1:F:98:TYR:HD1	1.43	0.83
1:B:65:LEU:HD23	3:B:234:HOH:O	1.81	0.81
1:G:142:GLU:HG2	1:G:146:LYS:HE3	1.64	0.80
1:F:36:LEU:HD21	1:F:41:ALA:HB2	1.63	0.79
1:H:7:VAL:HG13	1:H:36:LEU:HD22	1.65	0.78
1:H:23:GLU:HG3	1:H:33:VAL:HG21	1.66	0.78
1:H:36:LEU:HD21	1:H:41:ALA:HB2	1.68	0.75
1:F:124:LEU:HD11	1:F:126:MET:HE3	1.68	0.75
1:D:23:GLU:HG3	1:D:33:VAL:HG21	1.69	0.74
1:A:32:GLU:HG3	1:F:35:LEU:HD23	1.70	0.73
1:H:4:VAL:HB	1:H:33:VAL:HG12	1.69	0.72
1:D:124:LEU:HD11	1:D:126:MET:HE3	1.70	0.72
1:H:124:LEU:HD11	1:H:126:MET:CE	2.20	0.71
1:F:46:LEU:HB3	1:F:81:ILE:HG23	1.71	0.71
1:A:20:GLN:HG2	1:F:32:GLU:HG2	1.73	0.71
1:B:142:GLU:HG2	1:B:146:LYS:HE3	1.73	0.71
1:D:23:GLU:HG3	1:D:33:VAL:CG2	2.22	0.70
1:F:7:VAL:HG13	1:F:36:LEU:HD22	1.73	0.70
1:F:142:GLU:O	1:F:146:LYS:HG2	1.91	0.70
1:I:95:ASP:HB3	1:I:98:TYR:HD1	1.55	0.69
1:D:36:LEU:HD21	1:D:41:ALA:HB2	1.73	0.69
1:A:120:ILE:HB	1:A:147:GLN:HG3	1.73	0.68
1:B:16:GLU:O	1:B:20:GLN:HG3	1.92	0.68
1:E:58:SER:HB2	2:E:152:FMN:O4'	1.95	0.67
1:H:95:ASP:HB3	1:H:98:TYR:HD1	1.58	0.67
1:E:106:PRO:O	1:E:110:GLU:HG3	1.94	0.66
1:D:95:ASP:HB3	1:D:98:TYR:HD1	1.60	0.66
1:I:4:VAL:HB	1:I:33:VAL:HG12	1.78	0.66
1:D:36:LEU:CD2	1:D:41:ALA:HB2	2.26	0.65
1:F:54:LEU:HD22	1:F:89:ALA:HB3	1.79	0.65
1:D:126:MET:CE	1:D:136:ALA:HB3	2.27	0.64
1:H:46:LEU:HB3	1:H:81:ILE:HG23	1.78	0.64
1:I:23:GLU:HG3	1:I:33:VAL:HG21	1.79	0.63
1:D:95:ASP:HB3	1:D:98:TYR:CD1	2.33	0.63
1:B:142:GLU:O	1:B:146:LYS:HG2	1.98	0.63
1:E:2:SER:N	1:E:31:HIS:HD1	1.97	0.63
1:F:124:LEU:HD11	1:F:126:MET:CE	2.28	0.62
1:A:14:ASN:O	1:A:17:SER:HB3	2.00	0.62
1:F:124:LEU:HD21	1:F:126:MET:HE3	1.82	0.61
1:D:87:LYS:HB3	1:D:120:ILE:HG21	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:LEU:HB3	1:D:81:ILE:HG23	1.83	0.61
1:A:111:ARG:HD3	3:A:293:HOH:O	2.01	0.61
1:E:106:PRO:O	1:E:110:GLU:CG	2.49	0.60
1:H:23:GLU:HG3	1:H:33:VAL:CG2	2.31	0.60
1:A:36:LEU:HD13	1:A:41:ALA:HB2	1.82	0.60
1:H:124:LEU:HD11	1:H:126:MET:HE2	1.83	0.60
1:F:95:ASP:HB3	1:F:98:TYR:CD1	2.33	0.59
1:F:17:SER:HA	1:F:20:GLN:OE1	2.03	0.59
1:D:126:MET:HE2	1:D:133:ASP:HB3	1.85	0.59
1:H:47:ALA:HB1	1:H:86:ARG:HD3	1.84	0.59
1:H:142:GLU:O	1:H:146:LYS:HG2	2.03	0.59
1:D:142:GLU:O	1:D:146:LYS:HG2	2.03	0.58
1:I:36:LEU:HD21	1:I:41:ALA:HB2	1.85	0.58
1:H:44:GLU:HB2	1:H:80:ARG:NH2	2.19	0.58
1:B:36:LEU:HD22	1:B:37:ASN:O	2.03	0.58
1:G:36:LEU:HD22	1:G:37:ASN:O	2.02	0.58
1:F:131:SER:O	1:F:134:PRO:HD3	2.04	0.58
1:I:95:ASP:HB3	1:I:98:TYR:CD1	2.36	0.58
1:A:62:MET:O	1:A:64:ASP:N	2.37	0.58
1:H:124:LEU:CD2	1:H:126:MET:HE3	2.30	0.58
1:H:17:SER:HA	1:H:20:GLN:OE1	2.03	0.58
1:H:124:LEU:HD11	1:H:126:MET:HE3	1.85	0.58
1:B:23:GLU:HG3	1:B:33:VAL:HB	1.86	0.57
1:H:120:ILE:HB	1:H:147:GLN:HG3	1.85	0.57
1:F:36:LEU:CD2	1:F:41:ALA:HB2	2.31	0.57
1:I:126:MET:CE	1:I:136:ALA:HB3	2.34	0.57
1:G:106:PRO:O	1:G:110:GLU:HG3	2.04	0.57
1:F:126:MET:HE2	1:F:136:ALA:HB3	1.85	0.57
1:H:54:LEU:HD22	1:H:89:ALA:HB3	1.86	0.57
1:G:87:LYS:HB3	1:G:120:ILE:HG21	1.87	0.57
1:B:142:GLU:CG	1:B:146:LYS:HE3	2.36	0.56
1:F:39:ALA:HB2	1:F:70:ASP:CG	2.30	0.56
2:A:149:FMN:HM82	1:G:139:SER:HA	1.86	0.56
1:B:62:MET:O	1:B:64:ASP:N	2.38	0.56
1:I:142:GLU:O	1:I:146:LYS:HG2	2.05	0.56
1:A:106:PRO:O	1:A:110:GLU:HG3	2.04	0.56
1:F:36:LEU:HD23	1:F:37:ASN:O	2.05	0.56
1:F:3:LYS:HG2	1:F:32:GLU:HB2	1.88	0.55
1:H:39:ALA:HB2	1:H:70:ASP:CG	2.31	0.55
1:F:44:GLU:HB2	1:F:80:ARG:HH21	1.70	0.55
1:E:62:MET:O	1:E:64:ASP:N	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:MET:O	1:E:63:GLU:C	2.51	0.55
1:A:36:LEU:HD22	1:A:37:ASN:O	2.07	0.54
1:A:62:MET:O	1:A:63:GLU:C	2.50	0.54
1:B:135:GLU:CG	1:E:64:ASP:OD2	2.56	0.54
1:I:56:GLY:HA2	1:I:91:PHE:O	2.08	0.54
1:B:111:ARG:HH11	1:B:111:ARG:HG2	1.73	0.54
1:G:62:MET:O	1:G:64:ASP:N	2.40	0.54
1:G:6:ILE:HB	1:G:35:LEU:HD12	1.90	0.54
1:I:75:PHE:HA	1:I:78:PHE:CD1	2.43	0.53
1:B:110:GLU:O	1:B:114:GLU:HG3	2.07	0.53
1:I:26:ILE:HA	1:I:145:LEU:HD21	1.89	0.53
1:G:46:LEU:HB3	1:G:81:ILE:HG23	1.90	0.53
1:D:24:GLU:HG3	1:E:28:ALA:HB2	1.90	0.53
1:G:62:MET:O	1:G:63:GLU:C	2.51	0.53
1:A:95:ASP:HB3	1:A:98:TYR:HD1	1.73	0.53
1:B:64:ASP:O	1:B:66:GLU:N	2.42	0.53
1:D:60:TRP:CZ2	2:D:151:FMN:H5'2	2.43	0.53
1:I:54:LEU:HD22	1:I:89:ALA:HB3	1.89	0.53
1:B:65:LEU:HB2	1:B:72:LEU:CD2	2.39	0.53
1:E:75:PHE:HA	1:E:78:PHE:CD1	2.44	0.53
1:I:141:ALA:O	1:I:145:LEU:HG	2.09	0.53
1:A:64:ASP:O	1:A:66:GLU:N	2.42	0.52
1:E:87:LYS:HB3	1:E:120:ILE:HD13	1.91	0.52
1:F:110:GLU:O	1:F:114:GLU:HG3	2.10	0.52
1:B:62:MET:O	1:B:63:GLU:C	2.52	0.52
1:D:44:GLU:HB2	1:D:80:ARG:NH2	2.24	0.52
1:I:23:GLU:HG3	1:I:33:VAL:CG2	2.39	0.52
1:G:64:ASP:O	1:G:66:GLU:N	2.43	0.52
1:A:105:VAL:HB	1:A:106:PRO:CD	2.39	0.51
1:D:26:ILE:HA	1:D:145:LEU:HD21	1.92	0.51
1:E:16:GLU:O	1:E:20:GLN:HG3	2.11	0.51
1:D:110:GLU:O	1:D:114:GLU:HG3	2.10	0.51
1:H:95:ASP:HB3	1:H:98:TYR:CD1	2.41	0.51
1:E:67:MET:HE1	1:E:75:PHE:CD2	2.45	0.51
1:E:46:LEU:HB3	1:E:81:ILE:HG23	1.93	0.51
1:D:17:SER:OG	1:D:129:ASP:HB2	2.11	0.51
1:H:131:SER:O	1:H:134:PRO:HD3	2.10	0.51
1:I:139:SER:O	1:I:142:GLU:HB3	2.11	0.51
1:F:65:LEU:C	1:F:65:LEU:HD13	2.37	0.50
1:I:53:VAL:O	1:I:88:VAL:HA	2.10	0.50
1:E:62:MET:HB2	3:E:154:HOH:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:GLU:O	1:A:146:LYS:HG2	2.12	0.50
1:H:145:LEU:HD23	1:H:148:LEU:HD12	1.94	0.50
1:H:75:PHE:HA	1:H:78:PHE:CD1	2.47	0.49
1:E:36:LEU:HD12	1:E:46:LEU:HD11	1.93	0.49
1:E:58:SER:OG	1:E:60:TRP:NE1	2.43	0.49
1:G:14:ASN:O	1:G:18:ILE:HG13	2.13	0.49
1:D:36:LEU:C	1:D:36:LEU:HD23	2.38	0.49
1:G:62:MET:HB2	3:G:167:HOH:O	2.13	0.49
1:D:75:PHE:HA	1:D:78:PHE:CD1	2.48	0.49
1:A:75:PHE:HA	1:A:78:PHE:CD1	2.48	0.49
1:E:64:ASP:O	1:E:66:GLU:N	2.46	0.48
1:H:54:LEU:CD2	1:H:89:ALA:HB3	2.43	0.48
1:E:6:ILE:HB	1:E:35:LEU:HD12	1.96	0.48
1:F:5:LEU:HB2	1:F:50:TYR:CE2	2.48	0.48
1:D:11:SER:HB2	1:D:60:TRP:CZ2	2.48	0.48
1:G:8:PHE:CE1	1:G:16:GLU:HG3	2.48	0.48
1:A:62:MET:HB3	1:A:63:GLU:H	1.52	0.48
2:A:149:FMN:C8M	1:G:139:SER:HA	2.44	0.48
1:I:126:MET:HE2	1:I:136:ALA:HB3	1.96	0.48
1:G:3:LYS:NZ	3:G:155:HOH:O	2.46	0.48
1:D:3:LYS:HG2	1:D:32:GLU:HB2	1.95	0.48
1:E:87:LYS:HB3	1:E:120:ILE:HG21	1.95	0.48
1:G:56:GLY:HA2	1:G:91:PHE:O	2.14	0.48
1:A:95:ASP:HB3	1:A:98:TYR:CD1	2.49	0.47
1:H:65:LEU:C	1:H:65:LEU:HD13	2.39	0.47
1:B:111:ARG:HG2	1:B:111:ARG:NH1	2.29	0.47
1:G:65:LEU:HB2	1:G:72:LEU:CD2	2.44	0.47
1:I:36:LEU:C	1:I:36:LEU:HD23	2.39	0.47
1:A:19:ALA:HB1	1:A:35:LEU:HD11	1.95	0.47
1:B:111:ARG:HD3	3:B:172:HOH:O	2.13	0.47
1:A:59:ALA:HB3	2:A:149:FMN:C2	2.45	0.47
1:E:62:MET:HB3	1:E:63:GLU:H	1.48	0.47
1:H:87:LYS:HB3	1:H:120:ILE:HD13	1.95	0.47
1:F:91:PHE:CB	1:F:124:LEU:HB3	2.45	0.47
1:E:67:MET:HE1	1:E:75:PHE:CE2	2.50	0.46
1:I:88:VAL:HG12	1:I:89:ALA:N	2.30	0.46
1:D:87:LYS:HB3	1:D:120:ILE:HD13	1.97	0.46
1:F:47:ALA:HB1	1:F:86:ARG:HD3	1.97	0.46
1:H:91:PHE:CB	1:H:124:LEU:HB3	2.45	0.46
1:B:104:ALA:O	1:B:108:ILE:HG13	2.15	0.46
1:H:11:SER:HB2	1:H:60:TRP:CZ2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:21:LYS:CG	1:I:137:VAL:HG11	2.45	0.46
1:A:87:LYS:HB3	1:A:120:ILE:HG21	1.97	0.46
1:H:36:LEU:HD23	1:H:36:LEU:C	2.41	0.46
1:H:126:MET:HE2	1:H:136:ALA:CB	2.46	0.46
1:I:110:GLU:O	1:I:114:GLU:HG3	2.16	0.46
1:G:65:LEU:H	1:G:65:LEU:HG	1.34	0.46
1:F:56:GLY:HA2	1:F:91:PHE:O	2.16	0.46
1:E:110:GLU:O	1:E:114:GLU:HG3	2.16	0.45
1:H:56:GLY:HA2	1:H:91:PHE:O	2.16	0.45
1:G:113:LYS:HE2	1:G:119:ILE:CG1	2.46	0.45
1:G:142:GLU:O	1:G:146:LYS:HG2	2.16	0.45
1:F:44:GLU:HB2	1:F:80:ARG:NH2	2.30	0.45
1:B:35:LEU:HD12	1:B:35:LEU:HA	1.86	0.45
1:B:75:PHE:HA	1:B:78:PHE:CD1	2.52	0.45
1:F:87:LYS:HB3	1:F:120:ILE:HG21	1.99	0.45
1:B:62:MET:HB3	1:B:63:GLU:H	1.52	0.45
1:F:126:MET:HE2	1:F:136:ALA:CB	2.46	0.45
1:H:91:PHE:HB2	1:H:124:LEU:HD23	1.99	0.45
1:I:53:VAL:HG11	1:I:55:PHE:CZ	2.52	0.45
1:F:75:PHE:HA	1:F:78:PHE:CD1	2.52	0.45
1:B:21:LYS:HD2	1:B:21:LYS:HA	1.76	0.45
1:H:126:MET:HE1	1:H:137:VAL:HG23	1.99	0.45
1:D:18:ILE:HA	1:D:130:ALA:HB2	2.00	0.44
1:D:83:LEU:O	1:D:84:ALA:C	2.59	0.44
1:F:43:ALA:O	1:F:81:ILE:HA	2.17	0.44
1:B:106:PRO:O	1:B:110:GLU:CG	2.65	0.44
1:I:7:VAL:HA	1:I:36:LEU:O	2.18	0.44
1:I:101:PHE:HA	2:I:155:FMN:O2	2.18	0.44
1:B:72:LEU:HD12	1:B:72:LEU:O	2.17	0.44
1:A:111:ARG:HG2	1:A:111:ARG:HH11	1.83	0.44
1:D:23:GLU:HB2	1:D:35:LEU:HD22	1.99	0.44
1:H:7:VAL:HG13	1:H:36:LEU:CD2	2.43	0.44
1:H:36:LEU:HD23	1:H:37:ASN:C	2.41	0.44
1:E:23:GLU:HG3	1:E:33:VAL:HB	1.99	0.44
1:E:107:ALA:HA	1:E:110:GLU:OE1	2.17	0.44
1:B:120:ILE:HB	1:B:147:GLN:HG3	2.00	0.44
1:E:65:LEU:H	1:E:65:LEU:HG	1.37	0.44
1:I:78:PHE:HA	1:I:81:ILE:HD12	2.00	0.44
1:F:94:GLY:O	1:F:127:GLU:HG2	2.18	0.44
1:B:113:LYS:HE2	1:B:119:ILE:CG1	2.48	0.43
1:F:36:LEU:HD23	1:F:36:LEU:C	2.43	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:GLU:O	1:F:113:LYS:HG3	2.19	0.43
1:G:106:PRO:O	1:G:110:GLU:CG	2.66	0.43
1:D:3:LYS:HB3	1:D:3:LYS:HE3	1.75	0.43
1:F:91:PHE:HA	1:F:124:LEU:HB3	2.00	0.43
1:I:120:ILE:O	1:I:147:GLN:HG3	2.17	0.43
1:E:14:ASN:OD1	2:E:152:FMN:H5'1	2.19	0.43
1:E:111:ARG:HA	1:E:111:ARG:HD2	1.67	0.43
1:F:5:LEU:HB2	1:F:50:TYR:CZ	2.53	0.43
1:A:32:GLU:CG	1:F:35:LEU:HD23	2.44	0.43
1:G:65:LEU:HD12	1:G:72:LEU:HD21	2.01	0.43
1:E:35:LEU:HD12	1:E:35:LEU:HA	1.81	0.43
1:H:50:TYR:O	1:H:86:ARG:NH1	2.52	0.43
1:A:32:GLU:HG3	1:F:35:LEU:CD2	2.45	0.42
1:D:23:GLU:HG3	1:D:33:VAL:HG23	1.99	0.42
1:G:36:LEU:HD12	1:G:46:LEU:HD11	2.01	0.42
1:I:55:PHE:HB2	1:I:108:ILE:HG21	2.01	0.42
1:D:2:SER:HB3	1:D:51:ASP:OD2	2.18	0.42
1:H:104:ALA:O	1:H:108:ILE:HG13	2.19	0.42
1:H:126:MET:HE2	1:H:136:ALA:HB3	2.01	0.42
1:I:3:LYS:HE3	1:I:3:LYS:HB3	1.81	0.42
1:H:26:ILE:HA	1:H:145:LEU:HD21	2.01	0.42
1:H:109:GLU:O	1:H:113:LYS:HG3	2.19	0.42
1:G:87:LYS:HB3	1:G:120:ILE:CG2	2.48	0.42
1:F:124:LEU:CD1	1:F:126:MET:HE3	2.45	0.42
1:B:6:ILE:HB	1:B:35:LEU:HD12	2.00	0.42
1:B:135:GLU:HG3	1:E:64:ASP:OD2	2.20	0.42
1:I:46:LEU:HB3	1:I:81:ILE:HG23	2.02	0.42
1:A:36:LEU:HD12	1:A:46:LEU:HD11	2.01	0.42
1:A:65:LEU:H	1:A:65:LEU:HG	1.34	0.42
1:D:87:LYS:HB3	1:D:120:ILE:CG2	2.46	0.42
1:D:102:CYS:C	1:D:104:ALA:H	2.27	0.42
1:E:8:PHE:HB2	1:E:15:THR:HG22	2.01	0.42
1:E:8:PHE:HE2	1:E:35:LEU:HG	1.84	0.42
1:F:90:ALA:HB3	1:F:105:VAL:HG13	2.00	0.42
1:A:36:LEU:CD1	1:A:41:ALA:HB2	2.50	0.42
1:E:104:ALA:O	1:E:108:ILE:HG13	2.20	0.42
1:A:120:ILE:HB	1:A:147:GLN:CG	2.47	0.42
1:E:8:PHE:HA	1:E:56:GLY:O	2.19	0.42
1:I:68:GLN:OE1	1:I:70:ASP:HB2	2.20	0.41
1:F:144:VAL:O	1:F:148:LEU:HG	2.20	0.41
1:I:120:ILE:HD12	1:I:147:GLN:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:62:MET:HE2	1:H:62:MET:HB2	1.94	0.41
1:B:65:LEU:H	1:B:65:LEU:HG	1.35	0.41
1:G:62:MET:HB3	1:G:63:GLU:H	1.51	0.41
1:E:54:LEU:HD22	1:E:89:ALA:HB3	2.01	0.41
1:H:3:LYS:HG2	1:H:32:GLU:HB2	2.03	0.41
1:H:82:GLY:O	1:H:86:ARG:HD2	2.19	0.41
1:A:111:ARG:HD2	1:A:111:ARG:HA	1.80	0.41
1:B:93:SER:HA	1:B:126:MET:O	2.21	0.41
1:E:11:SER:HB2	1:E:60:TRP:CZ2	2.56	0.41
1:F:86:ARG:HH11	1:F:86:ARG:HG2	1.86	0.41
1:G:93:SER:HA	1:G:126:MET:O	2.20	0.41
1:E:62:MET:HE2	1:E:62:MET:HA	2.03	0.41
1:I:21:LYS:HG2	1:I:137:VAL:HG11	2.01	0.41
1:G:113:LYS:HE2	1:G:119:ILE:HG13	2.01	0.41
1:A:146:LYS:HA	1:A:146:LYS:HD3	1.86	0.41
1:D:126:MET:HE3	1:D:136:ALA:HB3	2.00	0.41
1:A:3:LYS:HE3	1:A:3:LYS:HB3	1.77	0.41
1:E:17:SER:OG	1:E:129:ASP:HB2	2.21	0.41
1:H:126:MET:HE1	1:H:137:VAL:CG2	2.51	0.41
1:H:145:LEU:HA	1:H:148:LEU:HD12	2.03	0.41
1:B:8:PHE:HE2	1:B:35:LEU:HG	1.86	0.40
1:A:54:LEU:HD22	1:A:89:ALA:HB3	2.03	0.40
1:I:120:ILE:HB	1:I:147:GLN:HG3	2.02	0.40
1:D:55:PHE:HB2	1:D:108:ILE:HG21	2.04	0.40
1:H:36:LEU:HD23	1:H:37:ASN:O	2.22	0.40
1:A:113:LYS:NZ	3:A:284:HOH:O	2.53	0.40
1:E:142:GLU:O	1:E:146:LYS:HG2	2.20	0.40
1:G:8:PHE:HA	1:G:56:GLY:O	2.21	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	145/148 (98%)	138 (95%)	3 (2%)	4 (3%)	4	6
1	B	145/148 (98%)	139 (96%)	2 (1%)	4 (3%)	4	6
1	D	145/148 (98%)	137 (94%)	8 (6%)	0	100	100
1	E	145/148 (98%)	140 (97%)	1 (1%)	4 (3%)	4	6
1	F	145/148 (98%)	138 (95%)	7 (5%)	0	100	100
1	G	145/148 (98%)	138 (95%)	2 (1%)	5 (3%)	3	4
1	H	145/148 (98%)	141 (97%)	4 (3%)	0	100	100
1	I	145/148 (98%)	139 (96%)	6 (4%)	0	100	100
All	All	1160/1184 (98%)	1110 (96%)	33 (3%)	17 (2%)	8	16

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLU
1	A	65	LEU
1	A	66	GLU
1	B	63	GLU
1	B	65	LEU
1	B	66	GLU
1	E	63	GLU
1	E	65	LEU
1	E	66	GLU
1	E	69	ASP
1	G	63	GLU
1	G	65	LEU
1	G	66	GLU
1	G	69	ASP
1	A	62	MET
1	G	62	MET
1	B	62	MET

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	110/111 (99%)	104 (94%)	6 (6%)	19	40
1	B	110/111 (99%)	104 (94%)	6 (6%)	19	40
1	D	110/111 (99%)	106 (96%)	4 (4%)	31	58
1	E	110/111 (99%)	104 (94%)	6 (6%)	19	40
1	F	110/111 (99%)	107 (97%)	3 (3%)	39	67
1	G	110/111 (99%)	104 (94%)	6 (6%)	19	40
1	H	110/111 (99%)	105 (96%)	5 (4%)	24	49
1	I	110/111 (99%)	107 (97%)	3 (3%)	39	67
All	All	880/888 (99%)	841 (96%)	39 (4%)	25	50

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	35	LEU
1	A	36	LEU
1	A	66	GLU
1	A	78	PHE
1	A	111	ARG
1	B	7	VAL
1	B	32	GLU
1	B	36	LEU
1	B	66	GLU
1	B	78	PHE
1	B	111	ARG
1	D	63	GLU
1	D	65	LEU
1	D	78	PHE
1	D	110	GLU
1	E	7	VAL
1	E	17	SER
1	E	36	LEU
1	E	72	LEU
1	E	78	PHE
1	E	131	SER
1	F	7	VAL
1	F	33	VAL
1	F	35	LEU
1	H	17	SER
1	H	33	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	63	GLU
1	H	78	PHE
1	H	110	GLU
1	I	63	GLU
1	I	78	PHE
1	I	110	GLU
1	G	7	VAL
1	G	36	LEU
1	G	66	GLU
1	G	69	ASP
1	G	78	PHE
1	G	111	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	147	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](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FMN	I	155	-	33,33,33	1.04	2 (6%)	48,50,50	1.20	7 (14%)
2	FMN	D	151	-	33,33,33	1.03	2 (6%)	48,50,50	1.20	6 (12%)
2	FMN	G	156	-	33,33,33	1.02	2 (6%)	48,50,50	1.33	8 (16%)
2	FMN	A	149	-	33,33,33	1.07	2 (6%)	48,50,50	1.25	7 (14%)
2	FMN	B	150	-	33,33,33	1.04	2 (6%)	48,50,50	1.32	6 (12%)
2	FMN	H	154	-	33,33,33	1.03	2 (6%)	48,50,50	1.24	7 (14%)
2	FMN	E	152	-	33,33,33	1.04	2 (6%)	48,50,50	1.65	11 (22%)
2	FMN	F	153	-	33,33,33	1.05	2 (6%)	48,50,50	1.26	7 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	I	155	-	-	7/18/18/18	0/3/3/3
2	FMN	D	151	-	-	4/18/18/18	0/3/3/3
2	FMN	G	156	-	-	4/18/18/18	0/3/3/3
2	FMN	A	149	-	-	4/18/18/18	0/3/3/3
2	FMN	B	150	-	-	4/18/18/18	0/3/3/3
2	FMN	H	154	-	-	5/18/18/18	0/3/3/3
2	FMN	E	152	-	-	3/18/18/18	0/3/3/3
2	FMN	F	153	-	-	4/18/18/18	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	149	FMN	C4A-N5	3.86	1.39	1.30
2	E	152	FMN	C4A-N5	3.76	1.38	1.30
2	F	153	FMN	C4A-N5	3.75	1.38	1.30
2	B	150	FMN	C4A-N5	3.71	1.38	1.30
2	H	154	FMN	C4A-N5	3.61	1.38	1.30
2	G	156	FMN	C4A-N5	3.60	1.38	1.30
2	I	155	FMN	C4A-N5	3.52	1.38	1.30
2	D	151	FMN	C4A-N5	3.43	1.38	1.30
2	D	151	FMN	C10-N1	2.81	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	155	FMN	C10-N1	2.67	1.38	1.33
2	A	149	FMN	C10-N1	2.62	1.38	1.33
2	B	150	FMN	C10-N1	2.44	1.38	1.33
2	E	152	FMN	C10-N1	2.39	1.38	1.33
2	H	154	FMN	C10-N1	2.36	1.38	1.33
2	G	156	FMN	C10-N1	2.31	1.37	1.33
2	F	153	FMN	C10-N1	2.28	1.37	1.33

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	152	FMN	C4'-C3'-C2'	-5.26	104.81	113.57
2	E	152	FMN	C4-N3-C2	-3.37	119.66	125.64
2	H	154	FMN	C4-N3-C2	-3.22	119.93	125.64
2	B	150	FMN	C4A-C10-N10	3.19	121.05	116.48
2	E	152	FMN	C4A-C10-N10	3.05	120.85	116.48
2	I	155	FMN	O4-C4-C4A	-3.03	118.52	126.53
2	G	156	FMN	C4A-C10-N10	3.01	120.78	116.48
2	B	150	FMN	O4-C4-C4A	-2.94	118.77	126.53
2	D	151	FMN	C4-N3-C2	-2.94	120.42	125.64
2	D	151	FMN	O4-C4-C4A	-2.91	118.85	126.53
2	F	153	FMN	C4-N3-C2	-2.89	120.51	125.64
2	G	156	FMN	O4-C4-C4A	-2.87	118.94	126.53
2	A	149	FMN	O4-C4-C4A	-2.86	118.97	126.53
2	A	149	FMN	C4-N3-C2	-2.82	120.63	125.64
2	E	152	FMN	C5'-C4'-C3'	2.82	117.53	112.22
2	H	154	FMN	C4A-C10-N10	2.80	120.49	116.48
2	F	153	FMN	C4A-C10-N10	2.79	120.48	116.48
2	B	150	FMN	C4-N3-C2	-2.79	120.70	125.64
2	E	152	FMN	O5'-C5'-C4'	-2.76	101.99	109.36
2	G	156	FMN	C4-N3-C2	-2.74	120.78	125.64
2	B	150	FMN	C10-C4A-N5	-2.73	119.24	124.81
2	A	149	FMN	C4A-C10-N10	2.70	120.34	116.48
2	E	152	FMN	O4-C4-C4A	-2.62	119.61	126.53
2	F	153	FMN	C10-C4A-N5	-2.61	119.47	124.81
2	G	156	FMN	O2P-P-O5'	2.60	113.46	106.67
2	F	153	FMN	O4-C4-C4A	-2.60	119.67	126.53
2	H	154	FMN	C4A-C4-N3	2.59	119.86	113.25
2	H	154	FMN	O4-C4-C4A	-2.59	119.69	126.53
2	E	152	FMN	C10-C4A-N5	-2.59	119.52	124.81
2	E	152	FMN	C4A-C4-N3	2.58	119.83	113.25
2	H	154	FMN	C10-C4A-N5	-2.58	119.54	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	155	FMN	C4-N3-C2	-2.55	121.11	125.64
2	I	155	FMN	C4A-C10-N10	2.54	120.11	116.48
2	A	149	FMN	C10-C4A-N5	-2.51	119.68	124.81
2	G	156	FMN	C9A-C5A-N5	-2.49	119.81	122.45
2	D	151	FMN	C4A-C4-N3	2.49	119.60	113.25
2	G	156	FMN	C10-C4A-N5	-2.48	119.75	124.81
2	F	153	FMN	C4A-C4-N3	2.47	119.54	113.25
2	A	149	FMN	C4A-C4-N3	2.45	119.49	113.25
2	D	151	FMN	C4A-C10-N10	2.39	119.91	116.48
2	I	155	FMN	C10-C4A-N5	-2.37	119.97	124.81
2	F	153	FMN	C9A-C5A-N5	-2.33	119.98	122.45
2	G	156	FMN	C5A-C9A-N10	2.31	120.05	117.97
2	D	151	FMN	C10-C4A-N5	-2.30	120.11	124.81
2	A	149	FMN	C9A-C5A-N5	-2.29	120.03	122.45
2	I	155	FMN	C9A-C5A-N5	-2.28	120.04	122.45
2	I	155	FMN	C5A-C9A-N10	2.27	120.02	117.97
2	I	155	FMN	C4A-C4-N3	2.27	119.03	113.25
2	D	151	FMN	C9A-C5A-N5	-2.27	120.05	122.45
2	A	149	FMN	C5A-C9A-N10	2.26	120.01	117.97
2	G	156	FMN	C4A-C4-N3	2.21	118.88	113.25
2	E	152	FMN	C9A-C5A-N5	-2.21	120.11	122.45
2	B	150	FMN	C4A-C4-N3	2.20	118.85	113.25
2	E	152	FMN	C5A-C9A-N10	2.19	119.95	117.97
2	H	154	FMN	C9A-C5A-N5	-2.18	120.14	122.45
2	E	152	FMN	O4'-C4'-C5'	-2.16	105.23	109.99
2	B	150	FMN	O3P-P-O5'	2.08	112.11	106.67
2	F	153	FMN	C5A-C9A-N10	2.06	119.83	117.97
2	H	154	FMN	C4A-C10-N1	-2.05	119.56	124.59

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	149	FMN	C1'-C2'-C3'-O3'
2	A	149	FMN	C1'-C2'-C3'-C4'
2	B	150	FMN	C1'-C2'-C3'-O3'
2	B	150	FMN	C1'-C2'-C3'-C4'
2	D	151	FMN	C1'-C2'-C3'-O3'
2	D	151	FMN	C1'-C2'-C3'-C4'
2	E	152	FMN	O4'-C4'-C5'-O5'
2	F	153	FMN	C1'-C2'-C3'-O3'
2	F	153	FMN	C1'-C2'-C3'-C4'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	H	154	FMN	C1'-C2'-C3'-O3'
2	H	154	FMN	C1'-C2'-C3'-C4'
2	I	155	FMN	C1'-C2'-C3'-O3'
2	I	155	FMN	C1'-C2'-C3'-C4'
2	I	155	FMN	C5'-O5'-P-O1P
2	G	156	FMN	C1'-C2'-C3'-O3'
2	G	156	FMN	C1'-C2'-C3'-C4'
2	A	149	FMN	O2'-C2'-C3'-C4'
2	B	150	FMN	O2'-C2'-C3'-C4'
2	G	156	FMN	O2'-C2'-C3'-C4'
2	A	149	FMN	O2'-C2'-C3'-O3'
2	G	156	FMN	O2'-C2'-C3'-O3'
2	D	151	FMN	O2'-C2'-C3'-C4'
2	H	154	FMN	O2'-C2'-C3'-C4'
2	I	155	FMN	O2'-C2'-C3'-C4'
2	F	153	FMN	O2'-C2'-C3'-C4'
2	E	152	FMN	C3'-C4'-C5'-O5'
2	D	151	FMN	O2'-C2'-C3'-O3'
2	H	154	FMN	O2'-C2'-C3'-O3'
2	I	155	FMN	O2'-C2'-C3'-O3'
2	B	150	FMN	O2'-C2'-C3'-O3'
2	I	155	FMN	C5'-O5'-P-O3P
2	F	153	FMN	O2'-C2'-C3'-O3'
2	H	154	FMN	C5'-O5'-P-O1P
2	E	152	FMN	C4'-C5'-O5'-P
2	I	155	FMN	C5'-O5'-P-O2P

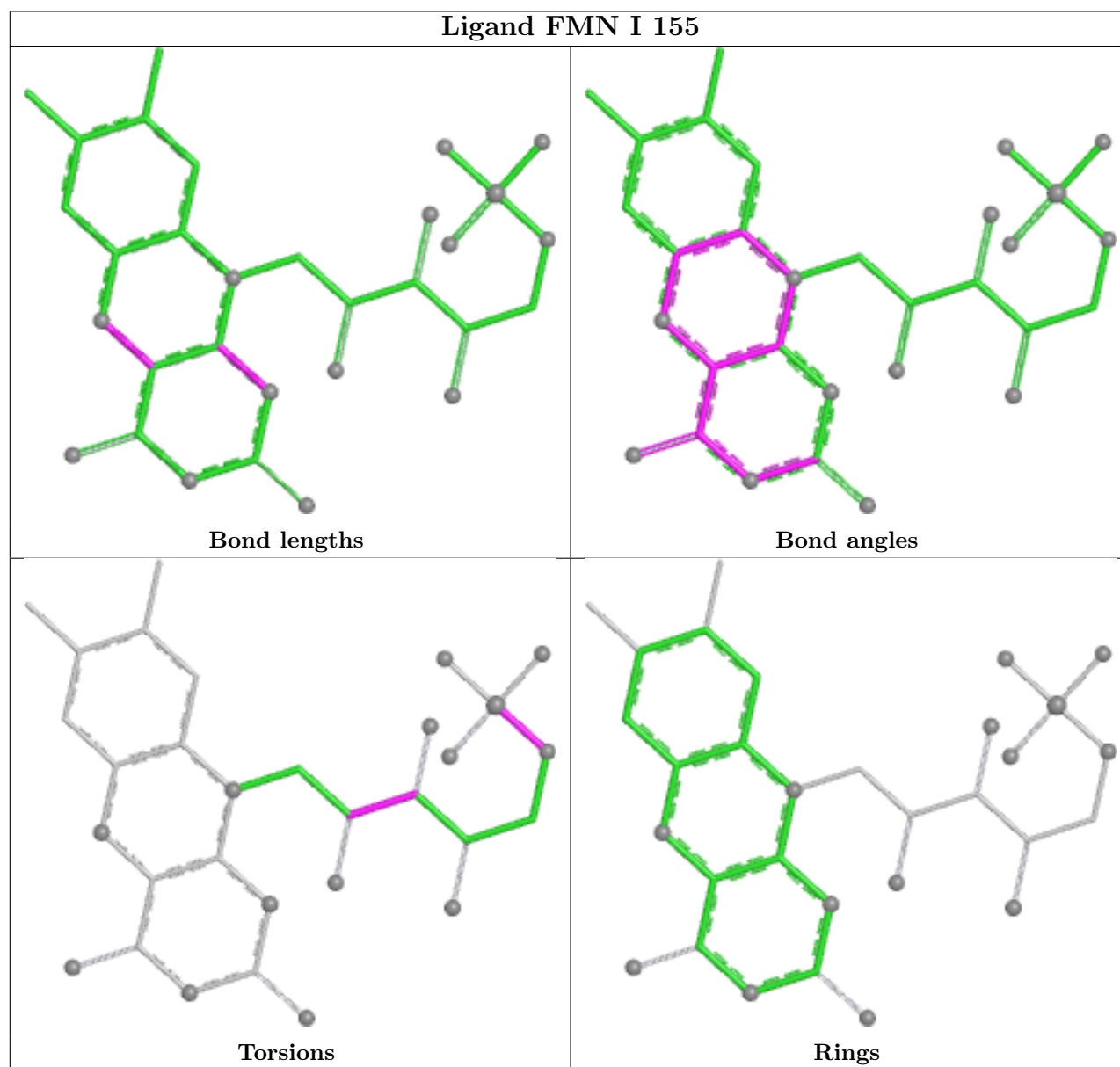
There are no ring outliers.

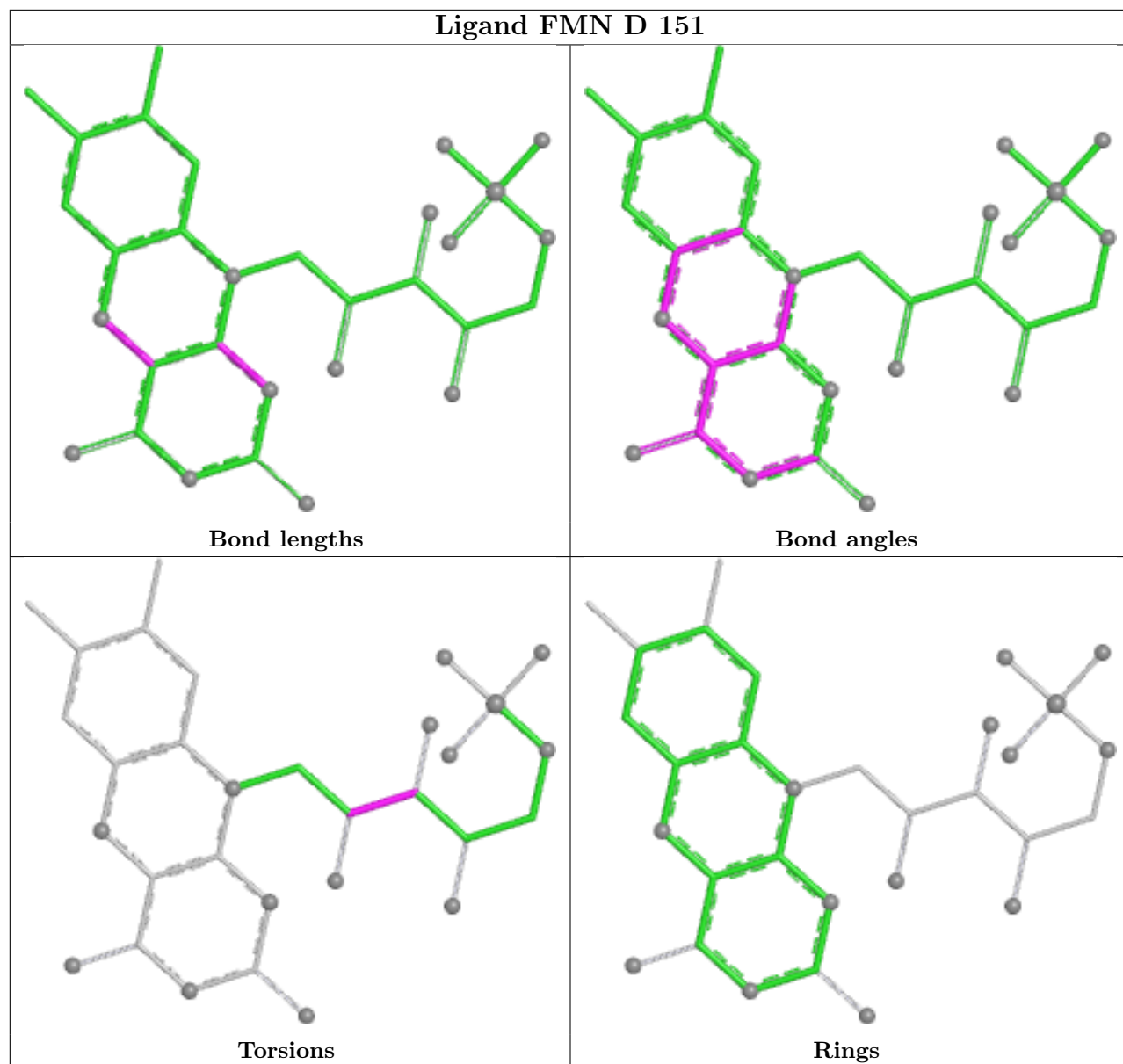
4 monomers are involved in 7 short contacts:

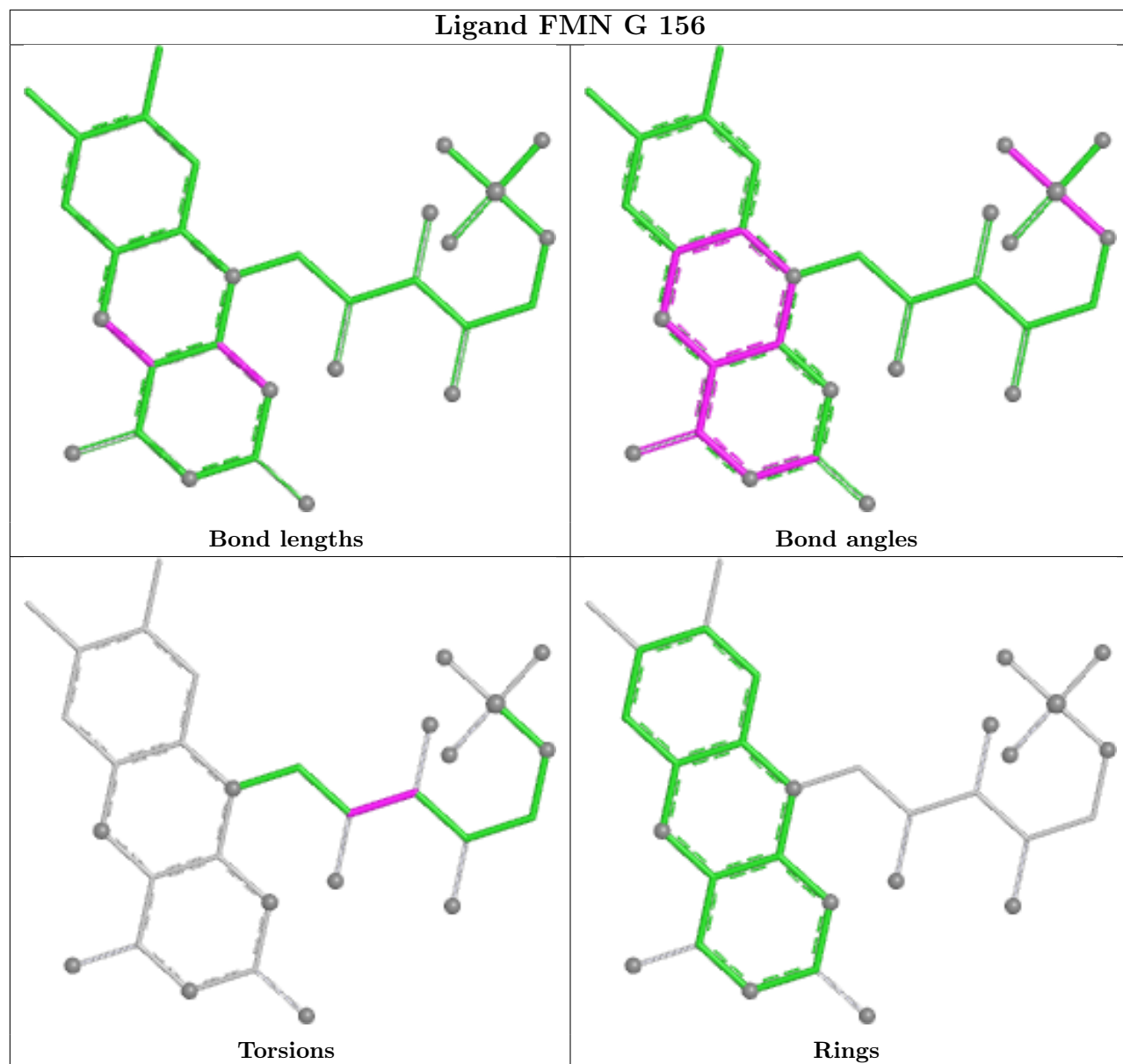
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	155	FMN	1	0
2	D	151	FMN	1	0
2	A	149	FMN	3	0
2	E	152	FMN	2	0

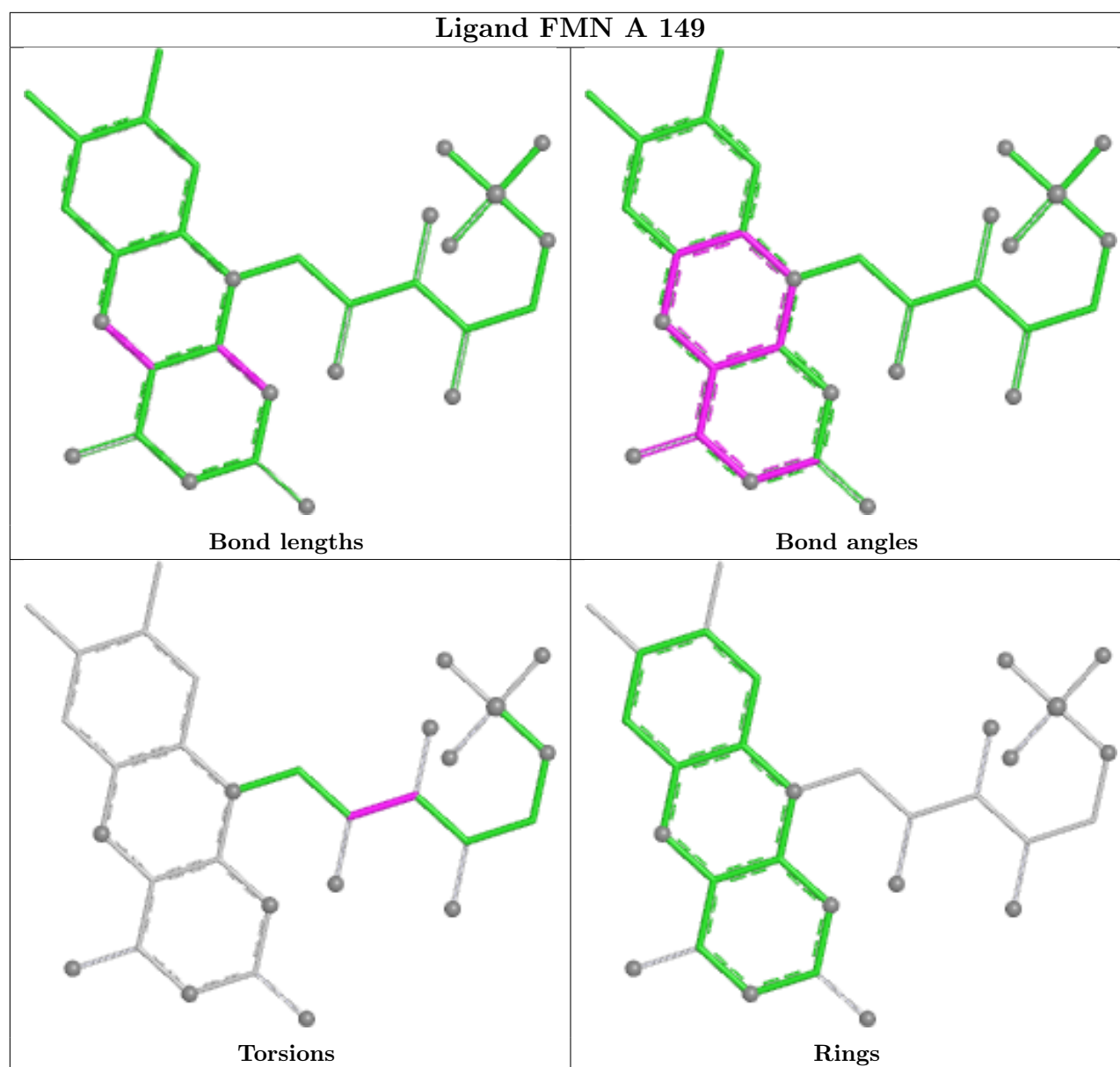
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

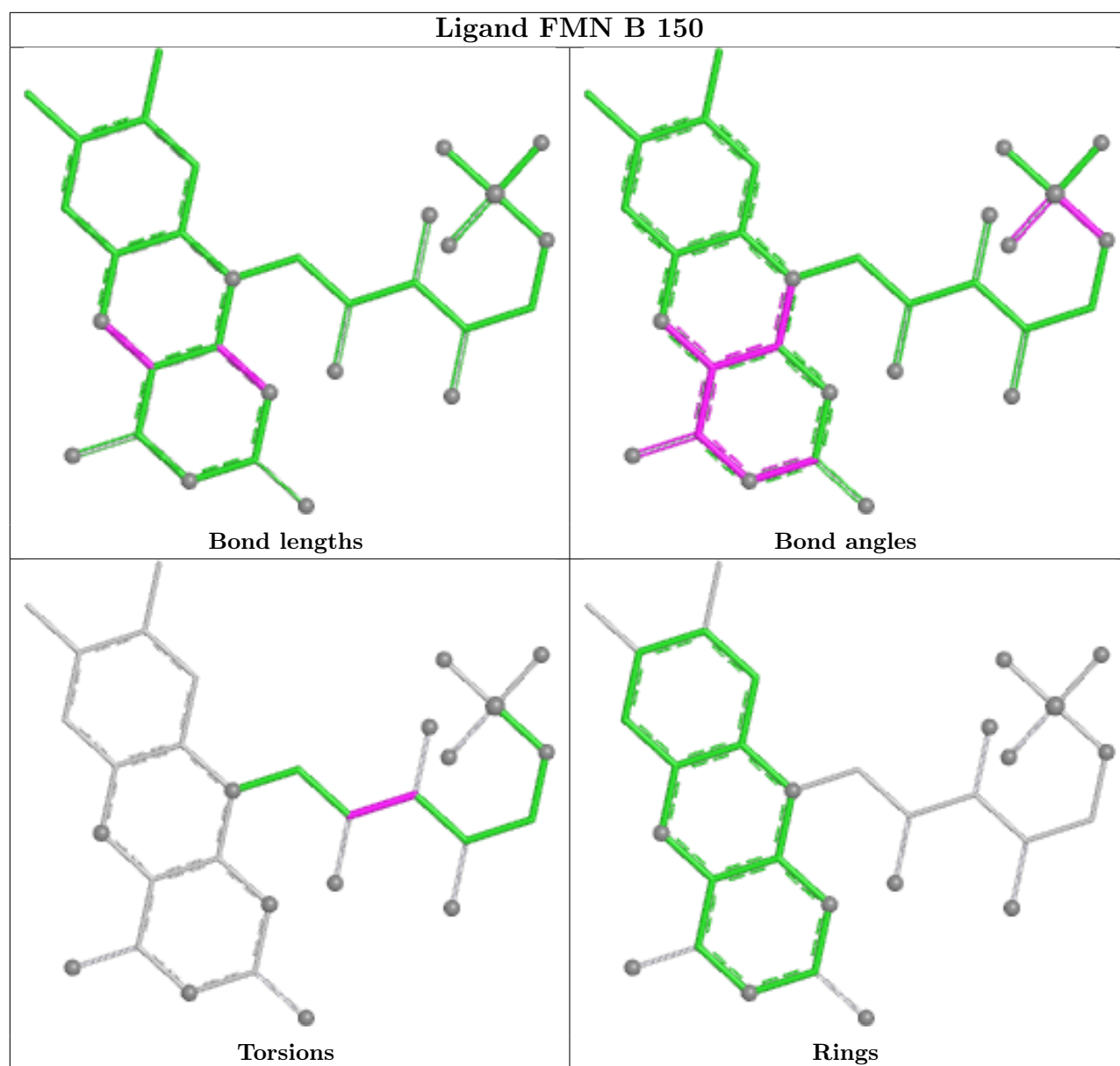
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

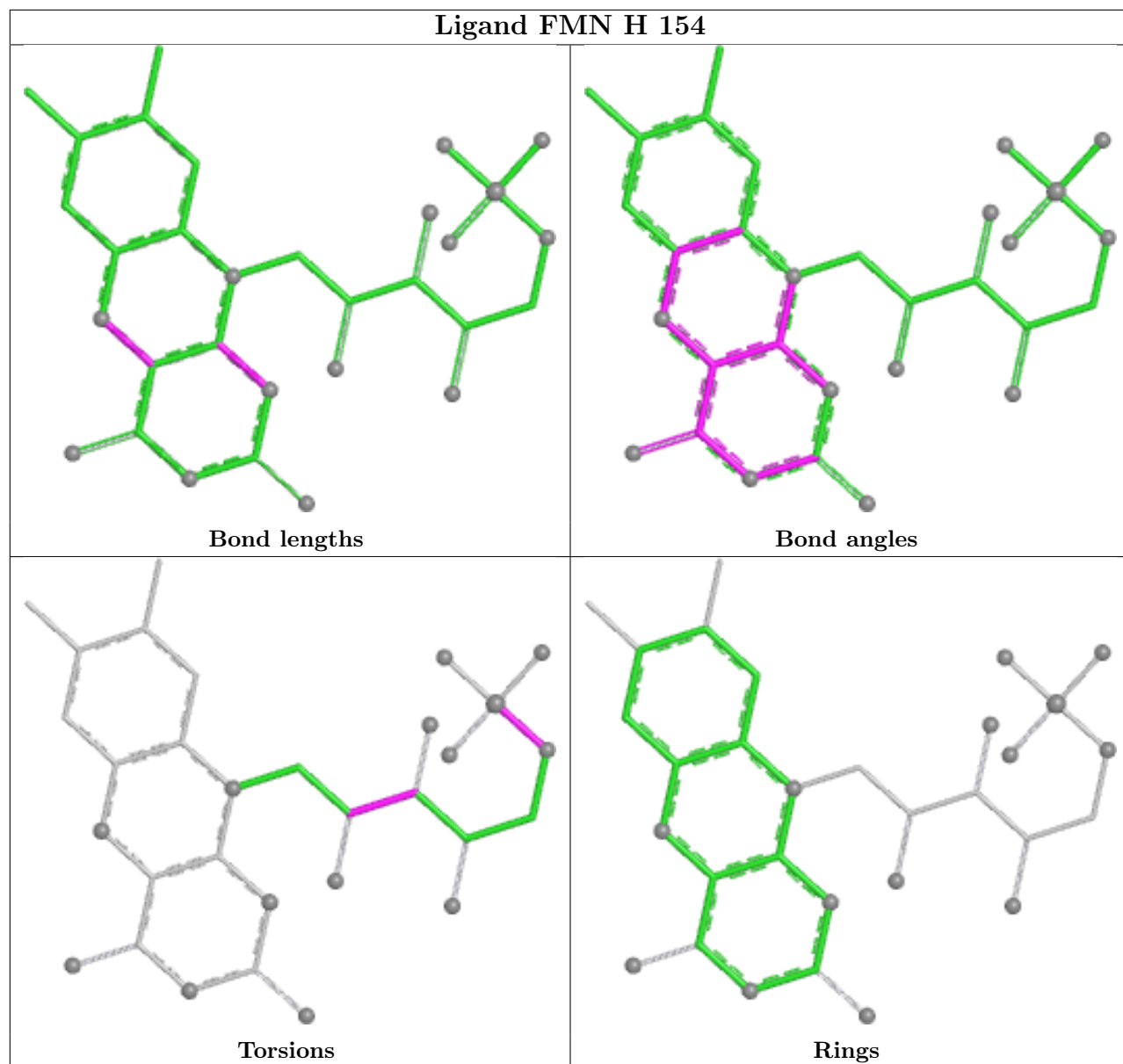


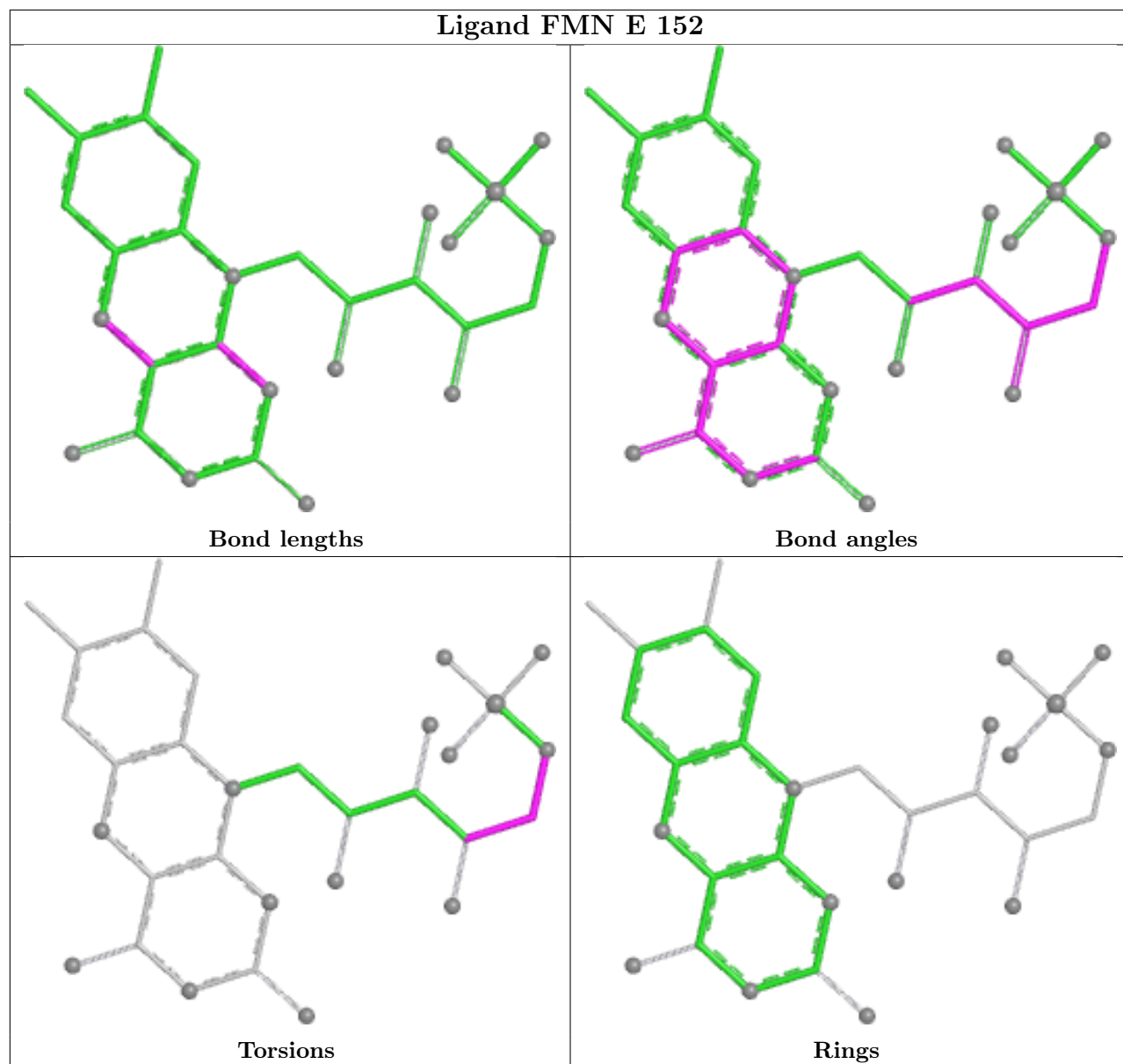


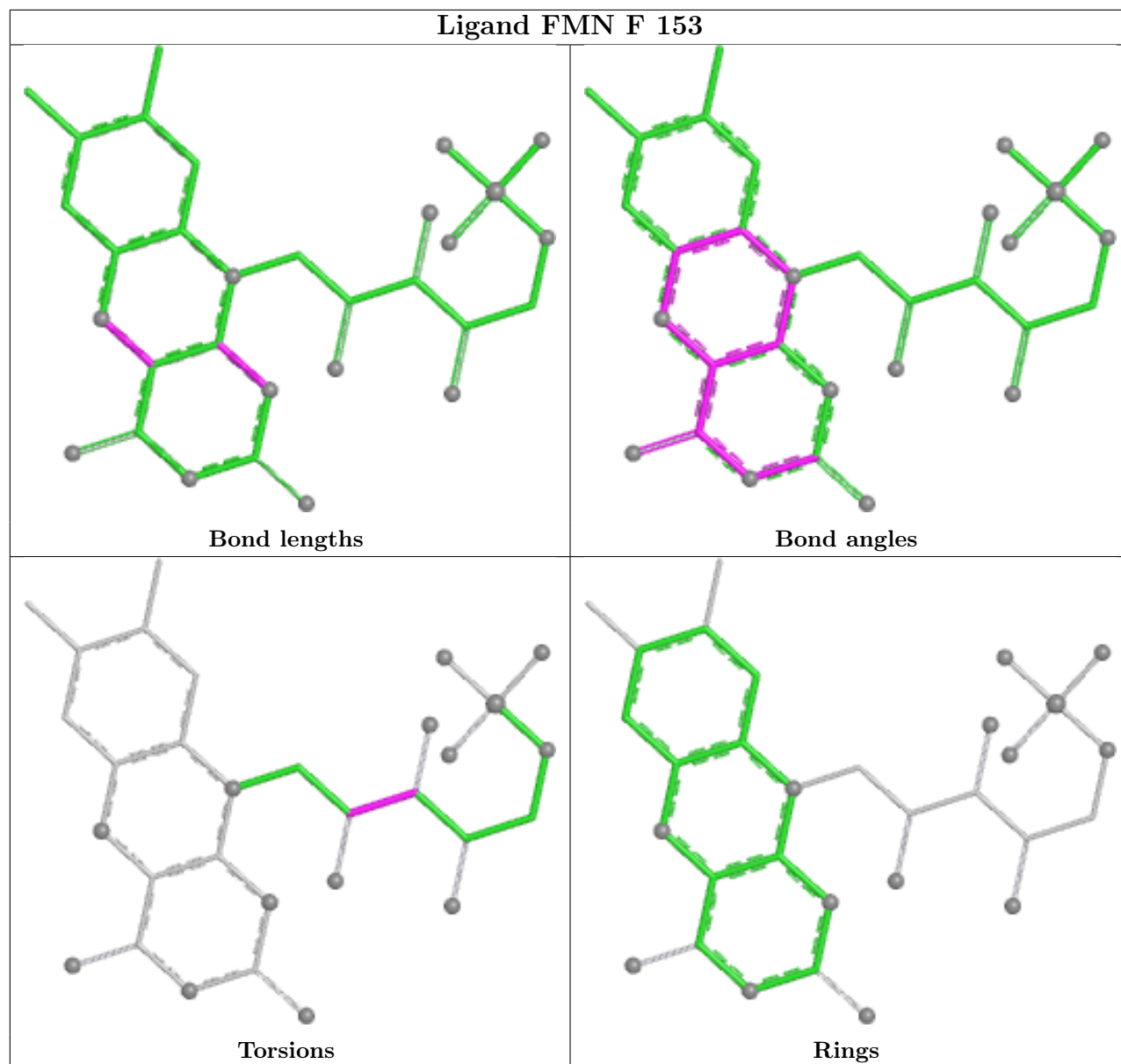












5.7 Other polymers [i](#)

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(Å²)	Q<0.9	
1	A	147/148 (99%)	8.04	147 (100%)	0	0	45, 56, 75, 107	0
1	B	147/148 (99%)	7.80	147 (100%)	0	0	45, 57, 74, 107	0
1	D	147/148 (99%)	10.15	147 (100%)	0	0	59, 71, 93, 114	0
1	E	147/148 (99%)	7.83	147 (100%)	0	0	45, 56, 74, 107	0
1	F	147/148 (99%)	9.85	147 (100%)	0	0	59, 70, 92, 114	0
1	G	147/148 (99%)	7.92	147 (100%)	0	0	46, 56, 74, 107	0
1	H	147/148 (99%)	10.03	147 (100%)	0	0	60, 70, 92, 114	0
1	I	147/148 (99%)	10.03	147 (100%)	0	0	59, 71, 92, 115	0
All	All	1176/1184 (99%)	8.96	1176 (100%)	0	0	45, 65, 89, 115	0

All (1176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	43	ALA	21.2
1	D	43	ALA	20.9
1	D	98	TYR	18.0
1	I	98	TYR	17.8
1	E	123	GLY	17.6
1	A	85	GLY	17.3
1	H	9	GLY	17.1
1	H	19	ALA	16.8
1	D	47	ALA	16.6
1	F	9	GLY	16.2
1	E	29	GLY	16.2
1	H	49	GLY	16.2
1	F	49	GLY	16.1
1	F	43	ALA	16.0
1	F	19	ALA	15.4
1	D	63	GLU	15.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	61	GLY	15.3
1	E	63	GLU	15.2
1	I	63	GLU	15.0
1	F	48	ASP	14.9
1	F	131	SER	14.9
1	I	47	ALA	14.8
1	I	132	ASN	14.7
1	E	64	ASP	14.5
1	F	134	PRO	14.4
1	D	8	PHE	14.4
1	D	101	PHE	14.3
1	H	42	SER	14.3
1	F	42	SER	14.2
1	H	134	PRO	14.2
1	H	48	ASP	14.2
1	I	61	GLY	14.1
1	I	101	PHE	14.0
1	H	131	SER	14.0
1	D	100	HIS	13.9
1	H	43	ALA	13.9
1	G	139	SER	13.9
1	F	4	VAL	13.8
1	D	69	ASP	13.7
1	B	64	ASP	13.6
1	D	132	ASN	13.6
1	B	63	GLU	13.5
1	G	63	GLU	13.5
1	H	130	ALA	13.5
1	F	25	LEU	13.4
1	I	81	ILE	13.4
1	I	8	PHE	13.4
1	I	2	SER	13.4
1	H	94	GLY	13.3
1	H	101	PHE	13.3
1	F	110	GLU	13.3
1	D	75	PHE	13.2
1	D	48	ASP	13.2
1	H	40	ASP	13.1
1	I	125	LYS	13.1
1	B	61	GLY	13.1
1	H	97	GLU	13.1
1	I	100	HIS	13.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	70	ASP	13.1
1	I	135	GLU	13.1
1	F	137	VAL	13.0
1	I	4	VAL	13.0
1	G	20	GLN	13.0
1	F	101	PHE	13.0
1	I	70	ASP	13.0
1	I	75	PHE	13.0
1	H	137	VAL	12.9
1	A	83	LEU	12.9
1	F	123	GLY	12.9
1	H	116	GLY	12.9
1	D	105	VAL	12.9
1	I	48	ASP	12.9
1	H	13	GLY	12.9
1	I	89	ALA	12.8
1	H	60	TRP	12.8
1	H	52	ALA	12.8
1	H	20	GLN	12.8
1	H	123	GLY	12.8
1	I	97	GLU	12.7
1	A	64	ASP	12.7
1	I	41	ALA	12.7
1	B	123	GLY	12.7
1	G	64	ASP	12.6
1	A	63	GLU	12.6
1	D	67	MET	12.6
1	I	44	GLU	12.5
1	I	92	ALA	12.5
1	F	10	SER	12.5
1	D	41	ALA	12.5
1	I	69	ASP	12.5
1	D	65	LEU	12.5
1	I	131	SER	12.5
1	D	44	GLU	12.4
1	D	42	SER	12.4
1	D	97	GLU	12.4
1	H	4	VAL	12.4
1	I	137	VAL	12.4
1	D	137	VAL	12.4
1	F	60	TRP	12.3
1	H	33	VAL	12.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	35	LEU	12.3
1	H	110	GLU	12.2
1	I	50	TYR	12.2
1	H	25	LEU	12.2
1	H	144	VAL	12.2
1	H	115	LEU	12.2
1	I	65	LEU	12.2
1	F	130	ALA	12.1
1	D	136	ALA	12.1
1	I	141	ALA	12.1
1	I	64	ASP	12.1
1	F	44	GLU	12.1
1	A	78	PHE	12.1
1	F	41	ALA	12.1
1	F	115	LEU	12.1
1	D	40	ASP	12.1
1	D	131	SER	12.1
1	I	78	PHE	12.0
1	H	18	ILE	12.0
1	D	114	GLU	12.0
1	H	65	LEU	12.0
1	A	61	GLY	12.0
1	D	81	ILE	12.0
1	D	141	ALA	12.0
1	I	76	GLU	11.9
1	I	54	LEU	11.9
1	D	93	SER	11.9
1	D	29	GLY	11.9
1	I	25	LEU	11.8
1	F	94	GLY	11.8
1	I	42	SER	11.8
1	I	67	MET	11.8
1	E	61	GLY	11.8
1	F	40	ASP	11.8
1	A	148	LEU	11.7
1	F	103	GLY	11.7
1	F	13	GLY	11.7
1	H	26	ILE	11.7
1	D	25	LEU	11.7
1	G	131	SER	11.7
1	H	100	HIS	11.7
1	A	44	GLU	11.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	138	ALA	11.7
1	D	50	TYR	11.6
1	H	56	GLY	11.6
1	F	11	SER	11.6
1	D	45	ASN	11.5
1	F	116	GLY	11.5
1	D	72	LEU	11.5
1	I	36	LEU	11.5
1	D	64	ASP	11.5
1	E	116	GLY	11.5
1	F	15	THR	11.4
1	F	97	GLU	11.4
1	F	118	THR	11.4
1	F	114	GLU	11.4
1	H	15	THR	11.4
1	B	85	GLY	11.4
1	F	144	VAL	11.4
1	D	95	ASP	11.4
1	H	118	THR	11.4
1	A	49	GLY	11.4
1	I	84	ALA	11.3
1	I	102	CYS	11.3
1	D	54	LEU	11.3
1	H	111	ARG	11.3
1	B	16	GLU	11.3
1	F	35	LEU	11.3
1	A	79	ASP	11.3
1	F	18	ILE	11.3
1	I	72	LEU	11.3
1	G	29	GLY	11.3
1	A	74	LEU	11.2
1	D	133	ASP	11.2
1	D	125	LYS	11.2
1	H	145	LEU	11.2
1	F	141	ALA	11.2
1	F	147	GLN	11.2
1	H	53	VAL	11.2
1	G	65	LEU	11.2
1	H	147	GLN	11.2
1	B	34	THR	11.2
1	D	2	SER	11.2
1	F	100	HIS	11.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	93	SER	11.2
1	G	18	ILE	11.2
1	F	57	CYS	11.1
1	D	142	GLU	11.1
1	D	78	PHE	11.1
1	F	84	ALA	11.1
1	F	16	GLU	11.0
1	I	79	ASP	11.0
1	D	76	GLU	11.0
1	H	78	PHE	11.0
1	I	51	ASP	11.0
1	D	60	TRP	11.0
1	D	90	ALA	11.0
1	I	114	GLU	11.0
1	D	68	GLN	11.0
1	E	84	ALA	11.0
1	D	79	ASP	10.9
1	H	35	LEU	10.9
1	I	45	ASN	10.9
1	B	82	GLY	10.9
1	H	57	CYS	10.9
1	H	58	SER	10.9
1	H	8	PHE	10.9
1	F	65	LEU	10.9
1	I	148	LEU	10.9
1	G	40	ASP	10.9
1	D	20	GLN	10.9
1	D	36	LEU	10.9
1	D	51	ASP	10.9
1	D	4	VAL	10.8
1	H	103	GLY	10.8
1	D	118	THR	10.8
1	A	112	ALA	10.8
1	H	27	ALA	10.8
1	I	105	VAL	10.8
1	D	92	ALA	10.8
1	F	111	ARG	10.8
1	I	60	TRP	10.8
1	B	20	GLN	10.8
1	B	27	ALA	10.7
1	H	17	SER	10.7
1	D	96	GLN	10.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	59	ALA	10.7
1	A	106	PRO	10.7
1	I	46	LEU	10.7
1	H	139	SER	10.7
1	D	102	CYS	10.7
1	H	142	GLU	10.7
1	H	29	GLY	10.7
1	G	14	ASN	10.7
1	B	9	GLY	10.6
1	G	34	THR	10.6
1	E	121	ALA	10.6
1	E	65	LEU	10.6
1	H	124	LEU	10.6
1	H	141	ALA	10.6
1	I	104	ALA	10.6
1	G	39	ALA	10.6
1	H	88	VAL	10.6
1	A	34	THR	10.6
1	A	113	LYS	10.6
1	I	39	ALA	10.6
1	D	112	ALA	10.6
1	A	65	LEU	10.5
1	D	62	MET	10.5
1	B	95	ASP	10.5
1	H	114	GLU	10.5
1	F	88	VAL	10.5
1	A	9	GLY	10.5
1	E	48	ASP	10.5
1	D	46	LEU	10.5
1	A	123	GLY	10.5
1	I	146	LYS	10.5
1	I	40	ASP	10.5
1	I	118	THR	10.5
1	G	80	ARG	10.5
1	D	148	LEU	10.5
1	H	61	GLY	10.4
1	E	80	ARG	10.4
1	F	78	PHE	10.4
1	I	15	THR	10.4
1	H	74	LEU	10.4
1	E	110	GLU	10.4
1	F	142	GLU	10.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	50	TYR	10.4
1	F	98	TYR	10.4
1	G	74	LEU	10.4
1	F	27	ALA	10.4
1	A	82	GLY	10.4
1	H	2	SER	10.4
1	H	98	TYR	10.4
1	F	8	PHE	10.4
1	F	138	ALA	10.4
1	F	20	GLN	10.4
1	F	83	LEU	10.4
1	D	59	ALA	10.3
1	E	117	ALA	10.3
1	G	41	ALA	10.3
1	I	62	MET	10.3
1	H	83	LEU	10.3
1	A	43	ALA	10.3
1	B	108	ILE	10.3
1	F	53	VAL	10.3
1	A	120	ILE	10.3
1	H	90	ALA	10.3
1	F	29	GLY	10.3
1	H	3	LYS	10.3
1	A	66	GLU	10.3
1	F	124	LEU	10.3
1	H	5	LEU	10.3
1	I	22	LEU	10.3
1	I	68	GLN	10.2
1	A	108	ILE	10.2
1	E	81	ILE	10.2
1	I	106	PRO	10.2
1	F	22	LEU	10.2
1	H	75	PHE	10.2
1	D	84	ALA	10.2
1	E	30	GLY	10.2
1	H	84	ALA	10.2
1	G	9	GLY	10.2
1	D	15	THR	10.2
1	I	20	GLN	10.2
1	G	98	TYR	10.2
1	I	95	ASP	10.1
1	H	34	THR	10.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	96	GLN	10.1
1	D	35	LEU	10.1
1	I	83	LEU	10.1
1	D	139	SER	10.1
1	D	91	PHE	10.1
1	A	141	ALA	10.1
1	B	59	ALA	10.1
1	D	37	ASN	10.1
1	I	99	GLU	10.1
1	F	90	ALA	10.0
1	F	7	VAL	10.0
1	E	60	TRP	10.0
1	D	103	GLY	10.0
1	H	135	GLU	10.0
1	H	93	SER	10.0
1	D	123	GLY	10.0
1	E	130	ALA	10.0
1	H	59	ALA	10.0
1	I	23	GLU	10.0
1	G	7	VAL	10.0
1	I	38	ALA	10.0
1	E	115	LEU	10.0
1	H	50	TYR	9.9
1	D	108	ILE	9.9
1	F	6	ILE	9.9
1	I	19	ALA	9.9
1	F	14	ASN	9.9
1	A	110	GLU	9.9
1	H	104	ALA	9.9
1	I	96	GLN	9.9
1	E	77	GLU	9.9
1	H	143	ASP	9.9
1	A	59	ALA	9.9
1	E	41	ALA	9.9
1	B	8	PHE	9.9
1	F	105	VAL	9.9
1	A	142	GLU	9.8
1	B	44	GLU	9.8
1	H	6	ILE	9.8
1	H	113	LYS	9.8
1	D	28	ALA	9.8
1	H	41	ALA	9.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	27	ALA	9.8
1	D	16	GLU	9.8
1	H	95	ASP	9.8
1	F	96	GLN	9.8
1	D	30	GLY	9.8
1	F	26	ILE	9.8
1	A	100	HIS	9.8
1	D	22	LEU	9.8
1	I	53	VAL	9.8
1	H	146	LYS	9.8
1	G	146	LYS	9.8
1	F	2	SER	9.8
1	D	135	GLU	9.7
1	I	86	ARG	9.7
1	D	57	CYS	9.7
1	F	56	GLY	9.7
1	D	27	ALA	9.7
1	G	42	SER	9.7
1	G	77	GLU	9.7
1	F	146	LYS	9.7
1	I	37	ASN	9.7
1	F	143	ASP	9.7
1	E	118	THR	9.7
1	F	47	ALA	9.7
1	I	91	PHE	9.7
1	G	33	VAL	9.6
1	H	16	GLU	9.6
1	F	104	ALA	9.6
1	E	146	LYS	9.6
1	D	124	LEU	9.6
1	F	75	PHE	9.6
1	F	113	LYS	9.6
1	I	87	LYS	9.6
1	D	111	ARG	9.6
1	E	40	ASP	9.6
1	F	119	ILE	9.6
1	I	26	ILE	9.6
1	E	39	ALA	9.6
1	F	59	ALA	9.6
1	H	14	ASN	9.6
1	A	20	GLN	9.6
1	G	61	GLY	9.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	129	ASP	9.6
1	D	26	ILE	9.6
1	E	72	LEU	9.6
1	I	5	LEU	9.6
1	D	39	ALA	9.6
1	I	117	ALA	9.6
1	G	19	ALA	9.6
1	I	71	PHE	9.5
1	A	30	GLY	9.5
1	B	130	ALA	9.5
1	A	146	LYS	9.5
1	I	134	PRO	9.5
1	B	132	ASN	9.5
1	D	94	GLY	9.5
1	F	12	THR	9.5
1	H	39	ALA	9.5
1	I	77	GLU	9.5
1	G	82	GLY	9.5
1	G	123	GLY	9.5
1	B	74	LEU	9.5
1	H	47	ALA	9.5
1	A	122	GLU	9.5
1	I	66	GLU	9.5
1	F	82	GLY	9.5
1	B	36	LEU	9.5
1	H	120	ILE	9.5
1	D	87	LYS	9.5
1	I	12	THR	9.4
1	I	111	ARG	9.4
1	B	78	PHE	9.4
1	A	45	ASN	9.4
1	H	10	SER	9.4
1	H	45	ASN	9.4
1	G	45	ASN	9.4
1	B	49	GLY	9.4
1	I	57	CYS	9.4
1	B	83	LEU	9.4
1	H	119	ILE	9.4
1	I	115	LEU	9.4
1	H	11	SER	9.4
1	F	145	LEU	9.4
1	H	12	THR	9.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	130	ALA	9.4
1	D	77	GLU	9.4
1	D	146	LYS	9.4
1	H	133	ASP	9.4
1	B	43	ALA	9.3
1	D	117	ALA	9.3
1	D	144	VAL	9.3
1	B	28	ALA	9.3
1	D	19	ALA	9.3
1	I	136	ALA	9.3
1	A	98	TYR	9.3
1	E	45	ASN	9.3
1	F	74	LEU	9.3
1	H	128	GLY	9.3
1	D	10	SER	9.3
1	H	69	ASP	9.3
1	D	130	ALA	9.3
1	B	65	LEU	9.3
1	H	64	ASP	9.3
1	D	49	GLY	9.3
1	F	128	GLY	9.3
1	I	74	LEU	9.3
1	G	72	LEU	9.3
1	A	139	SER	9.3
1	F	139	SER	9.3
1	F	132	ASN	9.2
1	E	119	ILE	9.2
1	I	32	GLU	9.2
1	F	95	ASP	9.2
1	A	84	ALA	9.2
1	E	144	VAL	9.2
1	A	50	TYR	9.2
1	D	66	GLU	9.2
1	I	110	GLU	9.2
1	B	24	GLU	9.2
1	D	31	HIS	9.2
1	E	108	ILE	9.2
1	H	96	GLN	9.2
1	F	52	ALA	9.2
1	B	72	LEU	9.2
1	I	94	GLY	9.2
1	A	24	GLU	9.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	99	GLU	9.2
1	G	81	ILE	9.2
1	G	78	PHE	9.1
1	I	127	GLU	9.1
1	I	28	ALA	9.1
1	B	142	GLU	9.1
1	H	37	ASN	9.1
1	F	79	ASP	9.1
1	E	136	ALA	9.1
1	D	83	LEU	9.1
1	H	105	VAL	9.1
1	D	106	PRO	9.1
1	D	12	THR	9.1
1	F	61	GLY	9.1
1	D	119	ILE	9.1
1	F	108	ILE	9.1
1	F	125	LYS	9.0
1	H	70	ASP	9.0
1	I	133	ASP	9.0
1	E	76	GLU	9.0
1	F	135	GLU	9.0
1	H	44	GLU	9.0
1	D	7	VAL	9.0
1	G	85	GLY	9.0
1	B	71	PHE	9.0
1	F	106	PRO	9.0
1	F	17	SER	9.0
1	H	73	SER	9.0
1	H	80	ARG	9.0
1	F	58	SER	9.0
1	B	110	GLU	9.0
1	F	24	GLU	9.0
1	D	74	LEU	9.0
1	E	74	LEU	9.0
1	D	53	VAL	9.0
1	B	40	ASP	9.0
1	E	95	ASP	9.0
1	H	63	GLU	9.0
1	G	16	GLU	9.0
1	E	31	HIS	9.0
1	F	31	HIS	9.0
1	H	102	CYS	9.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	147	GLN	9.0
1	H	82	GLY	9.0
1	I	49	GLY	9.0
1	I	103	GLY	9.0
1	D	140	PHE	8.9
1	B	23	GLU	8.9
1	F	64	ASP	8.9
1	B	35	LEU	8.9
1	D	104	ALA	8.9
1	A	105	VAL	8.9
1	D	33	VAL	8.9
1	I	108	ILE	8.9
1	A	111	ARG	8.9
1	F	45	ASN	8.9
1	E	113	LYS	8.9
1	A	115	LEU	8.9
1	I	11	SER	8.9
1	F	33	VAL	8.9
1	I	33	VAL	8.9
1	G	96	GLN	8.9
1	E	50	TYR	8.9
1	G	97	GLU	8.9
1	H	72	LEU	8.9
1	G	36	LEU	8.9
1	D	52	ALA	8.9
1	D	89	ALA	8.9
1	H	30	GLY	8.9
1	I	21	LYS	8.9
1	D	5	LEU	8.9
1	I	124	LEU	8.9
1	A	121	ALA	8.9
1	D	38	ALA	8.9
1	B	10	SER	8.9
1	A	118	THR	8.9
1	F	34	THR	8.9
1	H	7	VAL	8.9
1	D	6	ILE	8.8
1	D	113	LYS	8.8
1	F	3	LYS	8.8
1	A	48	ASP	8.8
1	B	121	ALA	8.8
1	E	106	PRO	8.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	85	GLY	8.8
1	B	101	PHE	8.8
1	D	71	PHE	8.8
1	I	14	ASN	8.8
1	D	115	LEU	8.8
1	H	92	ALA	8.8
1	E	131	SER	8.8
1	H	86	ARG	8.8
1	E	82	GLY	8.8
1	G	116	GLY	8.8
1	E	71	PHE	8.8
1	F	140	PHE	8.8
1	G	8	PHE	8.8
1	A	95	ASP	8.8
1	B	79	ASP	8.8
1	H	66	GLU	8.8
1	I	140	PHE	8.8
1	G	35	LEU	8.8
1	A	80	ARG	8.8
1	D	85	GLY	8.7
1	G	30	GLY	8.7
1	G	140	PHE	8.7
1	F	122	GLU	8.7
1	E	98	TYR	8.7
1	H	106	PRO	8.7
1	H	107	ALA	8.7
1	D	58	SER	8.7
1	E	2	SER	8.7
1	G	113	LYS	8.7
1	B	50	TYR	8.7
1	G	142	GLU	8.7
1	B	113	LYS	8.6
1	F	120	ILE	8.6
1	I	144	VAL	8.6
1	D	86	ARG	8.6
1	F	91	PHE	8.6
1	H	140	PHE	8.6
1	B	5	LEU	8.6
1	F	54	LEU	8.6
1	G	83	LEU	8.6
1	F	129	ASP	8.6
1	E	28	ALA	8.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	123	GLY	8.6
1	F	80	ARG	8.6
1	E	46	LEU	8.6
1	E	148	LEU	8.6
1	G	25	LEU	8.6
1	E	66	GLU	8.6
1	H	51	ASP	8.6
1	B	117	ALA	8.6
1	I	9	GLY	8.6
1	I	56	GLY	8.6
1	D	80	ARG	8.6
1	G	4	VAL	8.6
1	E	83	LEU	8.6
1	B	69	ASP	8.6
1	D	21	LYS	8.6
1	D	9	GLY	8.6
1	I	31	HIS	8.6
1	G	111	ARG	8.6
1	E	35	LEU	8.6
1	G	44	GLU	8.6
1	H	21	LYS	8.6
1	F	51	ASP	8.6
1	I	143	ASP	8.6
1	B	111	ARG	8.5
1	I	107	ALA	8.5
1	G	94	GLY	8.5
1	B	45	ASN	8.5
1	G	84	ALA	8.5
1	F	93	SER	8.5
1	B	106	PRO	8.5
1	F	99	GLU	8.5
1	G	110	GLU	8.5
1	F	37	ASN	8.5
1	F	70	ASP	8.5
1	E	59	ALA	8.5
1	F	28	ALA	8.5
1	I	52	ALA	8.5
1	B	73	SER	8.5
1	D	145	LEU	8.5
1	E	142	GLU	8.5
1	F	109	GLU	8.5
1	F	127	GLU	8.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	5	LEU	8.5
1	A	140	PHE	8.5
1	D	110	GLU	8.5
1	E	97	GLU	8.5
1	G	50	TYR	8.5
1	B	70	ASP	8.4
1	A	116	GLY	8.4
1	D	11	SER	8.4
1	B	133	ASP	8.4
1	F	39	ALA	8.4
1	F	102	CYS	8.4
1	G	21	LYS	8.4
1	A	27	ALA	8.4
1	E	47	ALA	8.4
1	G	27	ALA	8.4
1	D	23	GLU	8.4
1	D	24	GLU	8.4
1	F	86	ARG	8.4
1	H	148	LEU	8.4
1	G	46	LEU	8.4
1	H	62	MET	8.4
1	B	84	ALA	8.4
1	F	46	LEU	8.4
1	F	148	LEU	8.4
1	I	58	SER	8.4
1	B	146	LYS	8.4
1	D	14	ASN	8.4
1	B	119	ILE	8.4
1	E	27	ALA	8.4
1	G	10	SER	8.4
1	E	111	ARG	8.3
1	B	96	GLN	8.3
1	F	63	GLU	8.3
1	H	99	GLU	8.3
1	F	136	ALA	8.3
1	A	36	LEU	8.3
1	A	57	CYS	8.3
1	E	3	LYS	8.3
1	A	101	PHE	8.3
1	H	71	PHE	8.3
1	B	98	TYR	8.3
1	F	69	ASP	8.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	70	ASP	8.3
1	A	28	ALA	8.3
1	A	60	TRP	8.3
1	G	15	THR	8.3
1	H	91	PHE	8.3
1	G	48	ASP	8.3
1	D	134	PRO	8.3
1	F	72	LEU	8.3
1	H	22	LEU	8.3
1	G	60	TRP	8.3
1	A	86	ARG	8.3
1	H	127	GLU	8.2
1	I	16	GLU	8.2
1	D	56	GLY	8.2
1	F	133	ASP	8.2
1	G	95	ASP	8.2
1	B	37	ASN	8.2
1	E	14	ASN	8.2
1	E	107	ALA	8.2
1	D	116	GLY	8.2
1	I	113	LYS	8.2
1	E	129	ASP	8.2
1	B	76	GLU	8.2
1	D	32	GLU	8.2
1	F	66	GLU	8.2
1	H	32	GLU	8.2
1	A	3	LYS	8.2
1	B	57	CYS	8.2
1	E	42	SER	8.2
1	A	51	ASP	8.2
1	A	33	VAL	8.2
1	F	85	GLY	8.2
1	A	40	ASP	8.2
1	I	129	ASP	8.2
1	I	80	ARG	8.2
1	G	144	VAL	8.2
1	A	97	GLU	8.2
1	D	147	GLN	8.1
1	B	94	GLY	8.1
1	A	73	SER	8.1
1	H	132	ASN	8.1
1	G	132	ASN	8.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	88	VAL	8.1
1	E	44	GLU	8.1
1	F	32	GLU	8.1
1	F	62	MET	8.1
1	F	107	ALA	8.1
1	H	122	GLU	8.1
1	B	86	ARG	8.1
1	A	124	LEU	8.1
1	B	3	LYS	8.1
1	F	5	LEU	8.1
1	B	19	ALA	8.1
1	A	72	LEU	8.0
1	F	81	ILE	8.0
1	H	54	LEU	8.0
1	H	81	ILE	8.0
1	A	69	ASP	8.0
1	E	43	ALA	8.0
1	A	14	ASN	8.0
1	F	21	LYS	8.0
1	B	22	LEU	8.0
1	A	75	PHE	8.0
1	A	131	SER	8.0
1	E	34	THR	8.0
1	B	21	LYS	8.0
1	I	120	ILE	8.0
1	G	129	ASP	8.0
1	A	19	ALA	8.0
1	B	80	ARG	8.0
1	H	31	HIS	8.0
1	E	85	GLY	8.0
1	H	79	ASP	8.0
1	G	17	SER	8.0
1	A	132	ASN	8.0
1	B	128	GLY	7.9
1	D	120	ILE	7.9
1	G	120	ILE	7.9
1	B	97	GLU	7.9
1	D	18	ILE	7.9
1	F	55	PHE	7.9
1	E	147	GLN	7.9
1	F	73	SER	7.9
1	G	147	GLN	7.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	132	ASN	7.9
1	I	7	VAL	7.9
1	I	85	GLY	7.9
1	B	26	ILE	7.9
1	B	48	ASP	7.9
1	B	136	ALA	7.9
1	D	138	ALA	7.9
1	D	88	VAL	7.9
1	B	13	GLY	7.9
1	F	30	GLY	7.9
1	H	36	LEU	7.9
1	F	68	GLN	7.9
1	H	68	GLN	7.9
1	G	62	MET	7.9
1	G	69	ASP	7.8
1	B	47	ALA	7.8
1	D	121	ALA	7.8
1	G	71	PHE	7.8
1	E	36	LEU	7.8
1	F	87	LYS	7.8
1	A	92	ALA	7.8
1	H	117	ALA	7.8
1	I	112	ALA	7.8
1	E	100	HIS	7.8
1	A	4	VAL	7.8
1	D	127	GLU	7.8
1	G	108	ILE	7.8
1	B	141	ALA	7.8
1	D	107	ALA	7.8
1	E	78	PHE	7.8
1	H	55	PHE	7.8
1	B	77	GLU	7.8
1	A	71	PHE	7.8
1	A	117	ALA	7.8
1	B	66	GLU	7.7
1	B	144	VAL	7.7
1	I	88	VAL	7.7
1	I	116	GLY	7.7
1	G	6	ILE	7.7
1	E	96	GLN	7.7
1	F	92	ALA	7.7
1	H	121	ALA	7.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	136	ALA	7.7
1	H	125	LYS	7.7
1	A	7	VAL	7.7
1	G	73	SER	7.7
1	A	46	LEU	7.7
1	G	148	LEU	7.7
1	I	6	ILE	7.7
1	E	21	LYS	7.7
1	E	70	ASP	7.7
1	H	129	ASP	7.7
1	E	109	GLU	7.7
1	G	106	PRO	7.7
1	B	131	SER	7.7
1	A	119	ILE	7.7
1	G	134	PRO	7.7
1	A	94	GLY	7.7
1	G	90	ALA	7.6
1	I	55	PHE	7.6
1	B	88	VAL	7.6
1	G	124	LEU	7.6
1	B	18	ILE	7.6
1	I	119	ILE	7.6
1	E	86	ARG	7.6
1	I	142	GLU	7.6
1	B	46	LEU	7.6
1	D	73	SER	7.6
1	H	109	GLU	7.6
1	I	24	GLU	7.6
1	E	104	ALA	7.6
1	D	55	PHE	7.6
1	G	75	PHE	7.6
1	B	147	GLN	7.6
1	I	30	GLY	7.6
1	G	13	GLY	7.6
1	A	15	THR	7.6
1	E	69	ASP	7.6
1	H	89	ALA	7.6
1	B	55	PHE	7.6
1	A	5	LEU	7.6
1	E	105	VAL	7.6
1	G	49	GLY	7.6
1	B	134	PRO	7.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	130	ALA	7.5
1	E	90	ALA	7.5
1	I	130	ALA	7.5
1	G	117	ALA	7.5
1	B	25	LEU	7.5
1	A	18	ILE	7.5
1	B	12	THR	7.5
1	E	26	ILE	7.5
1	F	89	ALA	7.5
1	G	137	VAL	7.5
1	D	34	THR	7.5
1	F	71	PHE	7.5
1	A	2	SER	7.5
1	G	12	THR	7.5
1	G	136	ALA	7.5
1	A	114	GLU	7.5
1	D	82	GLY	7.5
1	E	137	VAL	7.5
1	I	82	GLY	7.5
1	G	101	PHE	7.4
1	G	24	GLU	7.4
1	E	33	VAL	7.4
1	I	73	SER	7.4
1	B	75	PHE	7.4
1	G	66	GLU	7.4
1	I	3	LYS	7.4
1	G	79	ASP	7.4
1	H	46	LEU	7.4
1	G	91	PHE	7.4
1	B	7	VAL	7.4
1	I	126	MET	7.4
1	G	119	ILE	7.4
1	D	128	GLY	7.4
1	A	10	SER	7.3
1	D	3	LYS	7.3
1	I	147	GLN	7.3
1	F	121	ALA	7.3
1	E	101	PHE	7.3
1	B	105	VAL	7.3
1	B	11	SER	7.3
1	B	42	SER	7.3
1	E	24	GLU	7.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	112	ALA	7.3
1	E	7	VAL	7.3
1	B	60	TRP	7.3
1	I	139	SER	7.3
1	H	24	GLU	7.3
1	A	52	ALA	7.3
1	E	19	ALA	7.3
1	I	145	LEU	7.3
1	A	90	ALA	7.3
1	E	120	ILE	7.3
1	A	145	LEU	7.2
1	F	126	MET	7.2
1	H	112	ALA	7.2
1	D	13	GLY	7.2
1	G	56	GLY	7.2
1	E	4	VAL	7.2
1	G	115	LEU	7.2
1	A	38	ALA	7.2
1	A	89	ALA	7.2
1	D	143	ASP	7.2
1	E	133	ASP	7.2
1	G	47	ALA	7.2
1	A	103	GLY	7.2
1	E	49	GLY	7.2
1	H	108	ILE	7.2
1	B	14	ASN	7.2
1	F	77	GLU	7.2
1	G	68	GLN	7.2
1	G	105	VAL	7.2
1	B	68	GLN	7.2
1	A	25	LEU	7.2
1	E	75	PHE	7.2
1	A	137	VAL	7.1
1	B	114	GLU	7.1
1	A	62	MET	7.1
1	H	126	MET	7.1
1	B	148	LEU	7.1
1	B	41	ALA	7.1
1	H	28	ALA	7.1
1	I	128	GLY	7.1
1	I	18	ILE	7.1
1	H	87	LYS	7.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	47	ALA	7.1
1	G	2	SER	7.1
1	G	121	ALA	7.1
1	I	109	GLU	7.1
1	A	129	ASP	7.1
1	B	38	ALA	7.1
1	E	9	GLY	7.1
1	A	16	GLU	7.1
1	A	76	GLU	7.1
1	G	37	ASN	7.1
1	G	112	ALA	7.1
1	E	94	GLY	7.1
1	A	134	PRO	7.0
1	H	23	GLU	7.0
1	E	18	ILE	7.0
1	G	53	VAL	7.0
1	I	34	THR	7.0
1	D	129	ASP	7.0
1	E	99	GLU	7.0
1	G	38	ALA	7.0
1	I	29	GLY	7.0
1	D	17	SER	7.0
1	I	122	GLU	7.0
1	A	133	ASP	7.0
1	E	112	ALA	7.0
1	H	76	GLU	6.9
1	G	135	GLU	6.9
1	A	136	ALA	6.9
1	G	133	ASP	6.9
1	E	20	GLN	6.9
1	G	26	ILE	6.9
1	G	58	SER	6.9
1	B	33	VAL	6.9
1	A	77	GLU	6.9
1	A	107	ALA	6.9
1	E	51	ASP	6.9
1	E	92	ALA	6.9
1	I	13	GLY	6.9
1	G	43	ALA	6.9
1	E	8	PHE	6.9
1	D	126	MET	6.9
1	F	23	GLU	6.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	77	GLU	6.9
1	A	53	VAL	6.8
1	A	88	VAL	6.8
1	B	81	ILE	6.8
1	A	35	LEU	6.8
1	I	121	ALA	6.8
1	E	62	MET	6.8
1	A	144	VAL	6.8
1	B	140	PHE	6.8
1	A	104	ALA	6.8
1	B	29	GLY	6.8
1	E	38	ALA	6.8
1	I	90	ALA	6.8
1	B	2	SER	6.8
1	G	93	SER	6.8
1	F	38	ALA	6.7
1	G	59	ALA	6.7
1	G	104	ALA	6.7
1	A	6	ILE	6.7
1	I	17	SER	6.7
1	B	62	MET	6.7
1	G	143	ASP	6.7
1	B	100	HIS	6.7
1	A	12	THR	6.7
1	E	141	ALA	6.7
1	B	109	GLU	6.7
1	E	15	THR	6.7
1	E	13	GLY	6.7
1	A	70	ASP	6.7
1	B	51	ASP	6.7
1	B	104	ALA	6.7
1	E	25	LEU	6.7
1	B	31	HIS	6.7
1	D	122	GLU	6.6
1	E	5	LEU	6.6
1	E	124	LEU	6.6
1	H	38	ALA	6.6
1	E	55	PHE	6.6
1	B	145	LEU	6.6
1	E	134	PRO	6.6
1	A	17	SER	6.6
1	A	58	SER	6.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	10	SER	6.6
1	A	135	GLU	6.6
1	G	3	LYS	6.6
1	B	135	GLU	6.6
1	G	127	GLU	6.6
1	B	137	VAL	6.6
1	E	79	ASP	6.5
1	E	122	GLU	6.5
1	E	23	GLU	6.5
1	B	116	GLY	6.5
1	G	92	ALA	6.5
1	B	32	GLU	6.5
1	G	122	GLU	6.5
1	E	52	ALA	6.4
1	B	143	ASP	6.4
1	A	102	CYS	6.4
1	B	124	LEU	6.4
1	G	118	THR	6.4
1	B	138	ALA	6.4
1	G	51	ASP	6.4
1	A	42	SER	6.3
1	E	68	GLN	6.3
1	F	117	ALA	6.3
1	A	93	SER	6.3
1	G	107	ALA	6.3
1	A	13	GLY	6.3
1	B	93	SER	6.3
1	E	10	SER	6.3
1	G	88	VAL	6.3
1	E	58	SER	6.2
1	E	102	CYS	6.2
1	D	109	GLU	6.2
1	E	17	SER	6.2
1	G	31	HIS	6.2
1	F	36	LEU	6.2
1	A	81	ILE	6.2
1	B	39	ALA	6.2
1	E	57	CYS	6.2
1	B	6	ILE	6.2
1	A	68	GLN	6.1
1	E	114	GLU	6.1
1	A	11	SER	6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	32	GLU	6.1
1	G	114	GLU	6.1
1	B	4	VAL	6.1
1	A	26	ILE	6.1
1	A	55	PHE	6.1
1	A	143	ASP	6.1
1	A	8	PHE	6.1
1	G	141	ALA	6.1
1	E	16	GLU	6.1
1	B	56	GLY	6.0
1	G	145	LEU	6.0
1	A	87	LYS	6.0
1	G	28	ALA	6.0
1	B	58	SER	6.0
1	G	11	SER	6.0
1	G	54	LEU	6.0
1	A	29	GLY	6.0
1	A	109	GLU	6.0
1	G	125	LYS	5.9
1	E	125	LYS	5.9
1	B	17	SER	5.9
1	G	100	HIS	5.9
1	G	23	GLU	5.9
1	A	41	ALA	5.9
1	A	31	HIS	5.9
1	G	86	ARG	5.9
1	E	91	PHE	5.8
1	E	135	GLU	5.8
1	A	21	LYS	5.8
1	A	56	GLY	5.8
1	E	87	LYS	5.8
1	B	52	ALA	5.8
1	E	143	ASP	5.8
1	E	93	SER	5.8
1	B	126	MET	5.8
1	G	89	ALA	5.7
1	B	122	GLU	5.7
1	B	139	SER	5.7
1	A	22	LEU	5.7
1	B	115	LEU	5.7
1	B	112	ALA	5.7
1	E	140	PHE	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	126	MET	5.7
1	A	54	LEU	5.7
1	I	138	ALA	5.7
1	G	55	PHE	5.7
1	G	52	ALA	5.6
1	B	30	GLY	5.6
1	E	37	ASN	5.6
1	B	120	ILE	5.6
1	G	57	CYS	5.6
1	E	11	SER	5.6
1	E	103	GLY	5.6
1	G	128	GLY	5.6
1	E	6	ILE	5.6
1	B	99	GLU	5.5
1	E	73	SER	5.5
1	B	118	THR	5.5
1	G	76	GLU	5.5
1	B	91	PHE	5.5
1	A	91	PHE	5.5
1	B	15	THR	5.5
1	E	128	GLY	5.5
1	A	32	GLU	5.5
1	E	145	LEU	5.5
1	F	67	MET	5.4
1	B	107	ALA	5.4
1	B	92	ALA	5.4
1	B	67	MET	5.4
1	A	39	ALA	5.4
1	A	67	MET	5.4
1	B	102	CYS	5.4
1	A	99	GLU	5.4
1	G	87	LYS	5.3
1	B	125	LYS	5.3
1	G	99	GLU	5.3
1	A	125	LYS	5.3
1	E	12	THR	5.3
1	A	37	ASN	5.2
1	E	67	MET	5.1
1	E	22	LEU	5.1
1	E	53	VAL	5.1
1	E	138	ALA	5.1
1	A	128	GLY	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	138	ALA	5.1
1	B	90	ALA	5.1
1	B	127	GLU	5.0
1	F	76	GLU	5.0
1	G	22	LEU	5.0
1	E	32	GLU	4.9
1	E	89	ALA	4.9
1	H	67	MET	4.9
1	G	67	MET	4.8
1	E	139	SER	4.8
1	G	138	ALA	4.8
1	A	126	MET	4.7
1	B	89	ALA	4.7
1	G	102	CYS	4.7
1	B	87	LYS	4.7
1	G	109	GLU	4.6
1	B	53	VAL	4.6
1	G	103	GLY	4.5
1	A	127	GLU	4.5
1	B	103	GLY	4.4
1	A	23	GLU	4.2
1	E	126	MET	4.2
1	E	56	GLY	4.1
1	B	54	LEU	3.9
1	E	127	GLU	3.8
1	E	54	LEU	3.4

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](#)

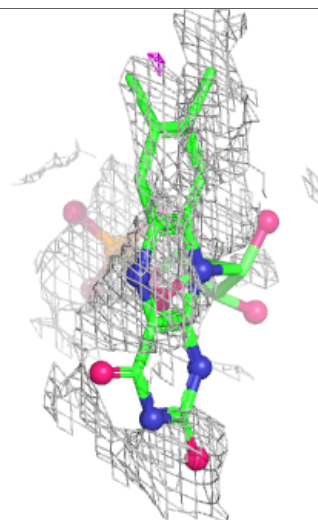
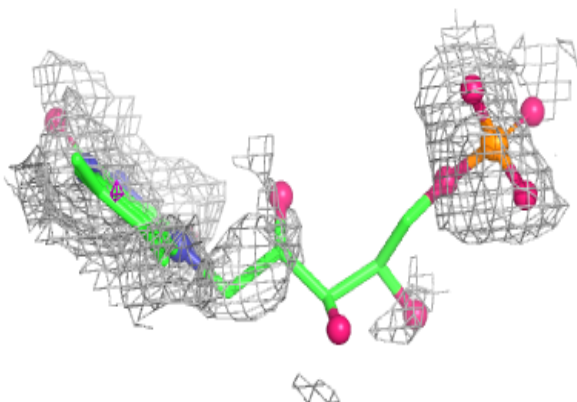
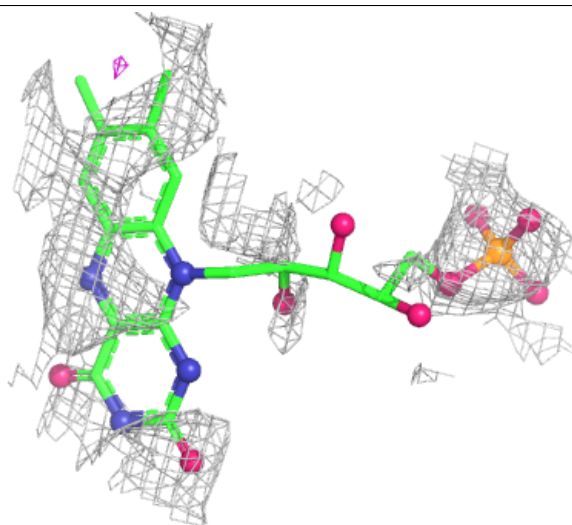
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	FMN	D	151	31/31	0.29	0.50	73,82,86,87	0
2	FMN	I	155	31/31	0.34	0.47	74,84,86,88	0
2	FMN	F	153	31/31	0.35	0.47	69,74,76,80	0
2	FMN	H	154	31/31	0.41	0.46	66,75,77,80	0
2	FMN	B	150	31/31	0.72	0.39	55,58,63,69	0
2	FMN	A	149	31/31	0.73	0.39	56,60,63,71	0
2	FMN	E	152	31/31	0.74	0.40	56,60,63,71	0
2	FMN	G	156	31/31	0.74	0.37	54,58,63,70	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.

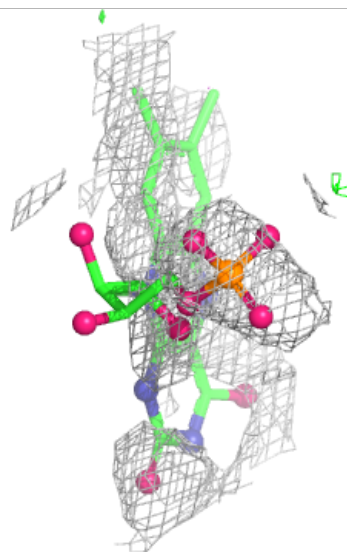
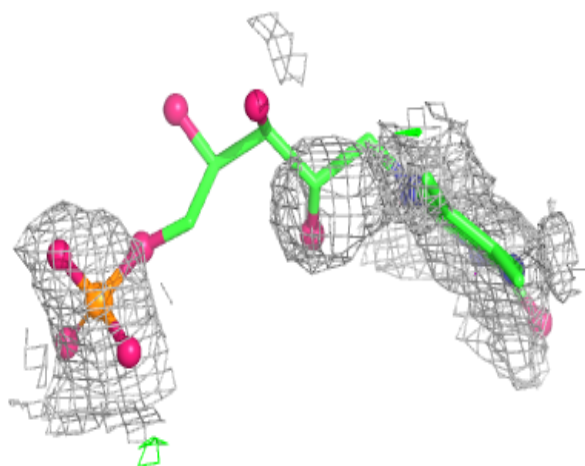
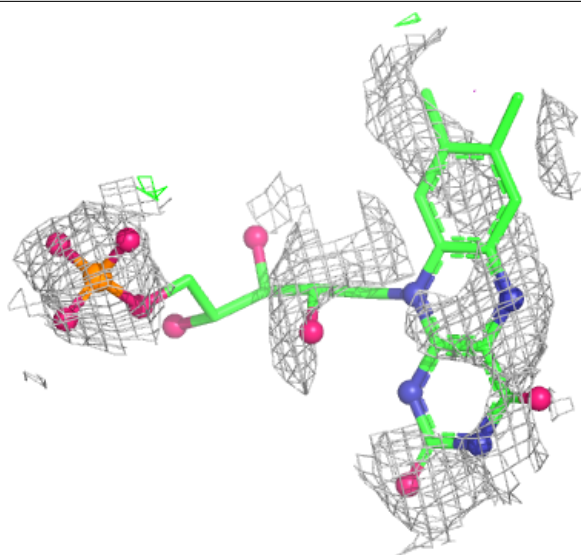
Electron density around FMN D 151:

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



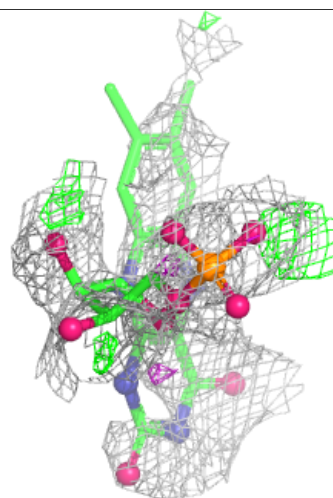
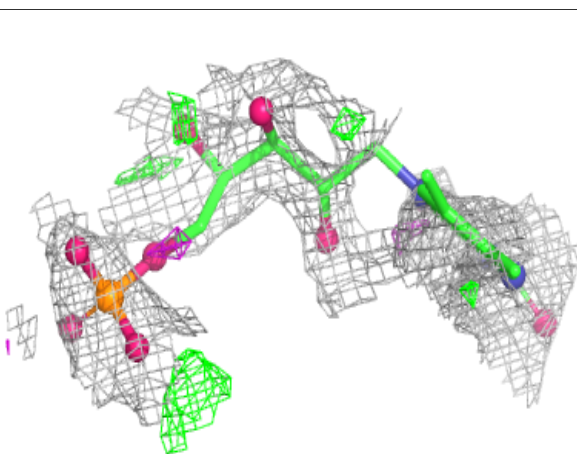
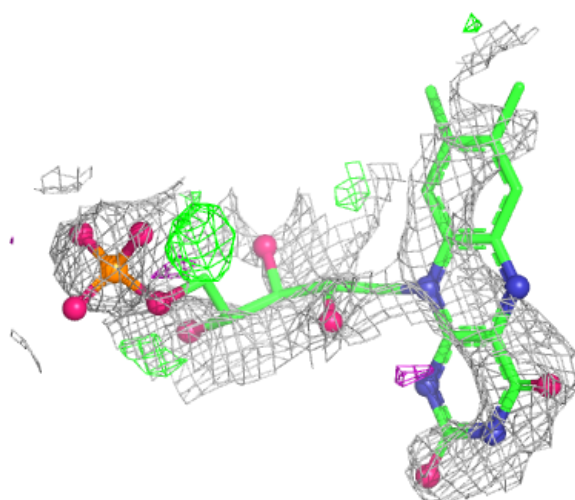
Electron density around FMN I 155:

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



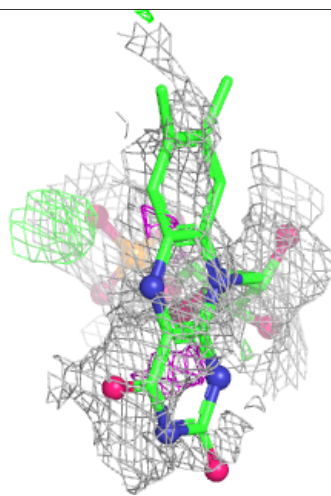
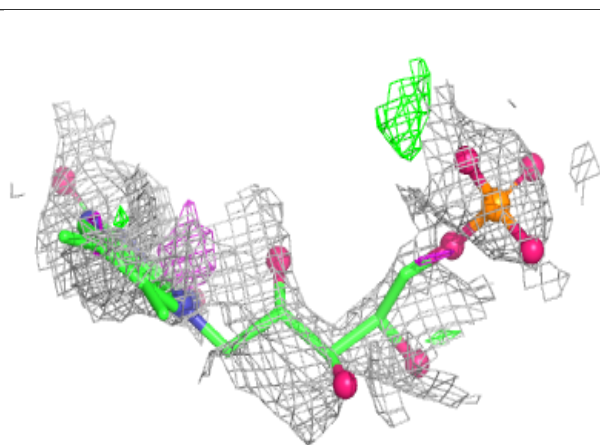
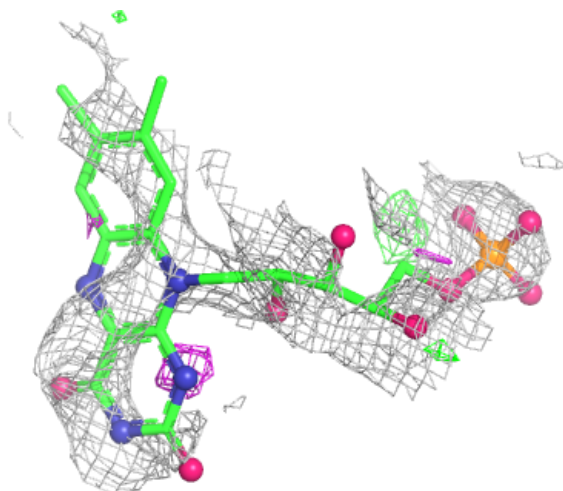
Electron density around FMN F 153:

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



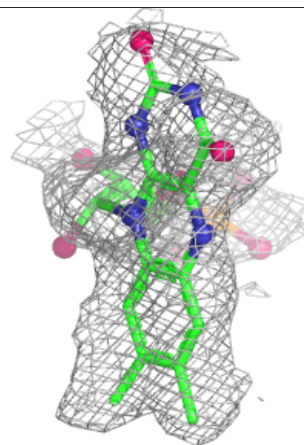
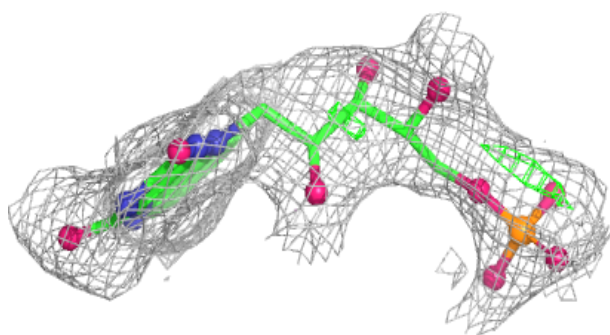
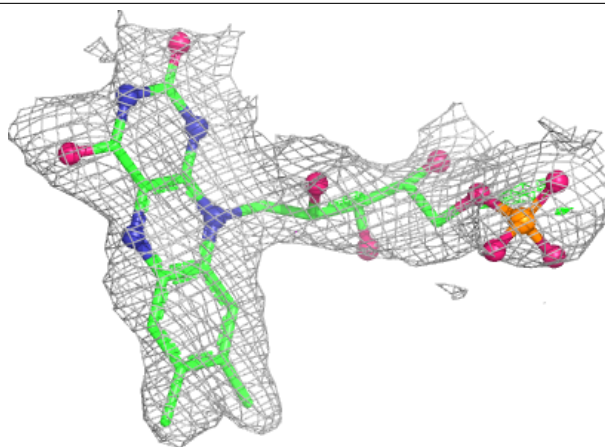
Electron density around FMN H 154:

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



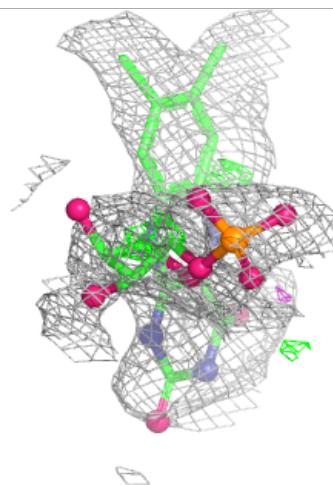
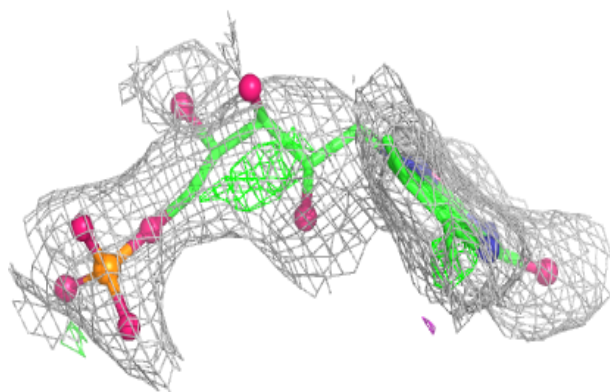
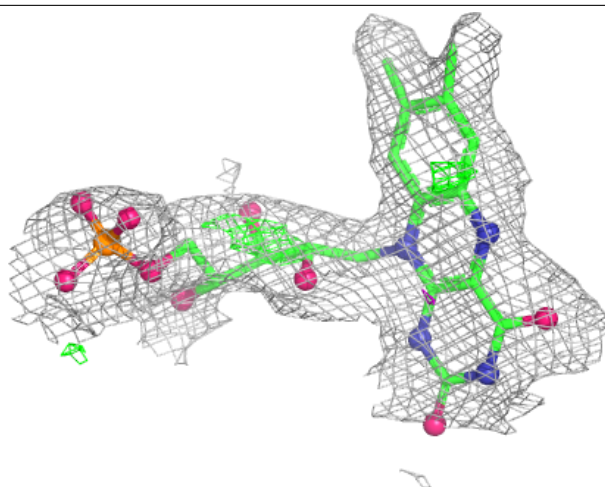
Electron density around FMN B 150:

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



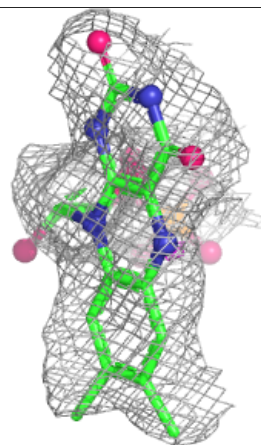
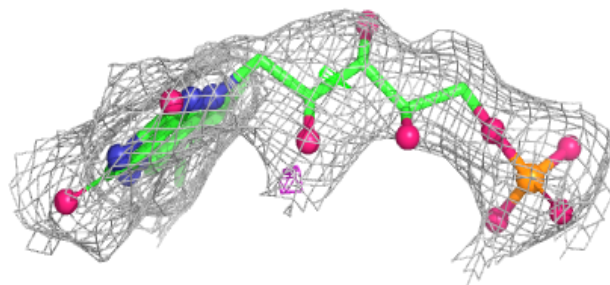
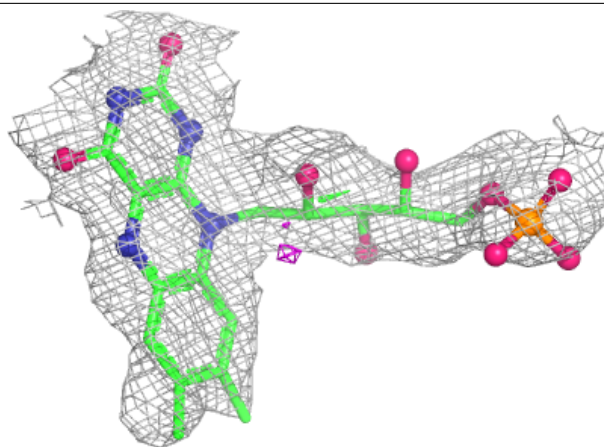
Electron density around FMN A 149:

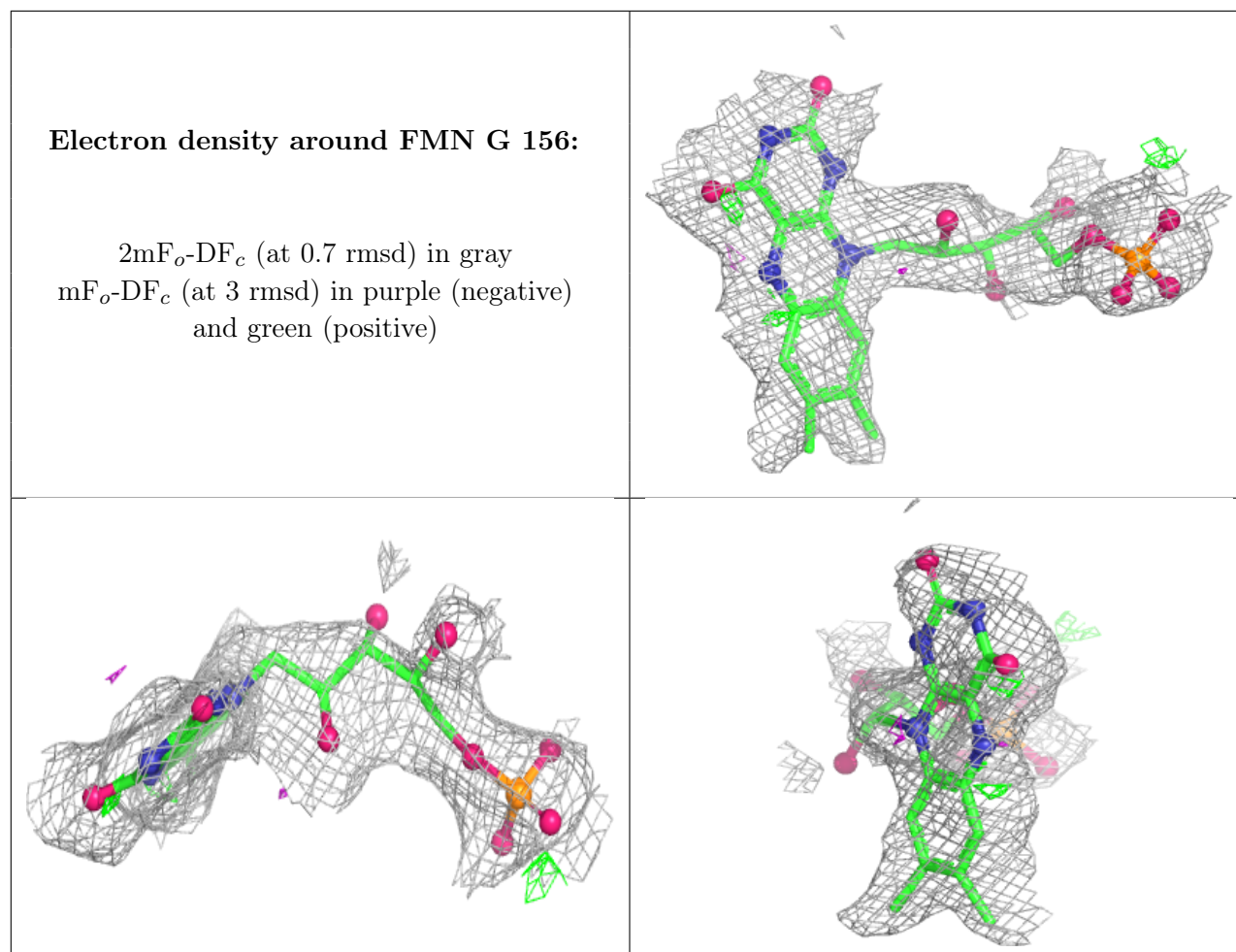
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMN E 152:

$2mF_o - DF_c$ (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.