



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:36 PM UTC

PDB ID : 6DVH / pdb_00006dvh
Title : Lactate Monooxygenase from Mycobacterium smegmatis - C203A mutant
Authors : Kean, K.M.; Karplus, P.A.
Deposited on : 2018-06-23
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

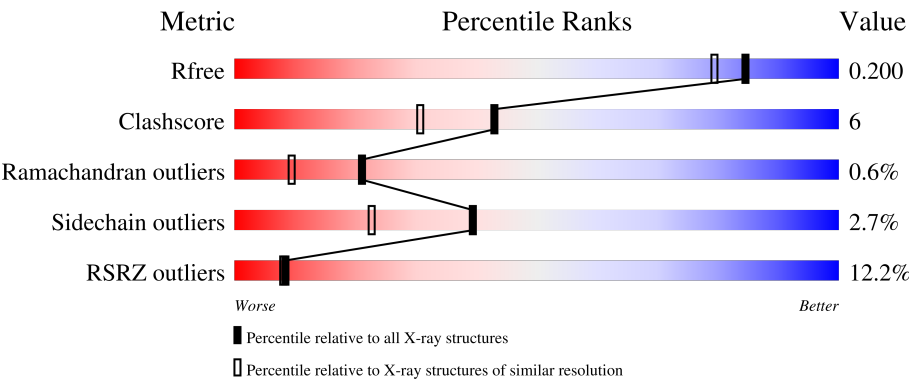
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	394	91% 8% .
1	B	394	7% 90% 9% ..
1	C	394	92% 6% .
1	D	394	8% 86% 13% .
1	E	394	25% 86% 13% .

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Mol	Chain	Length	Quality of chain
1	F	394	32% 84% 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20104 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.

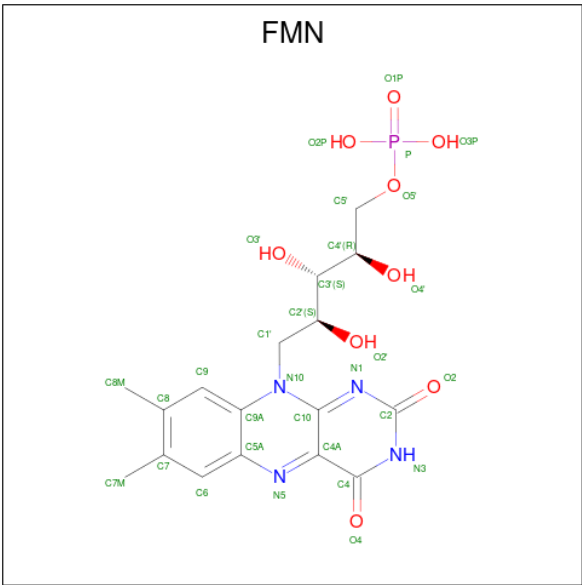
- Molecule 1 is a protein called Lactate 2-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	12	0
			3080	1964	533	571	12			
1	B	394	Total	C	N	O	S	0	22	0
			3166	2020	548	586	12			
1	C	394	Total	C	N	O	S	0	7	0
			3066	1949	540	565	12			
1	D	394	Total	C	N	O	S	0	7	0
			3062	1949	535	566	12			
1	E	394	Total	C	N	O	S	0	6	0
			3043	1935	530	566	12			
1	F	393	Total	C	N	O	S	0	6	0
			3037	1933	529	564	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	ALA	CYS	engineered mutation	UNP P21795
B	203	ALA	CYS	engineered mutation	UNP P21795
C	203	ALA	CYS	engineered mutation	UNP P21795
D	203	ALA	CYS	engineered mutation	UNP P21795
E	203	ALA	CYS	engineered mutation	UNP P21795
F	203	ALA	CYS	engineered mutation	UNP P21795

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	1
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	1
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	1
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

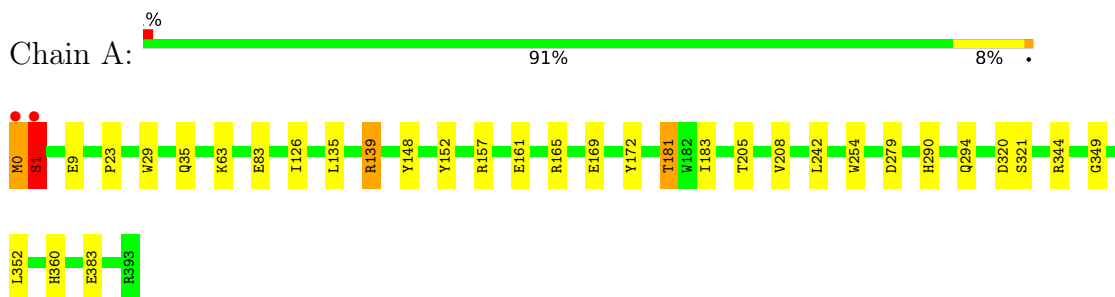
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	499	Total	O	0	4
			499	499		
4	B	358	Total	O	0	4
			358	358		
4	C	313	Total	O	0	2
			313	313		
4	D	182	Total	O	0	2
			182	182		
4	E	13	Total	O	0	0
			13	13		
4	F	9	Total	O	0	0
			9	9		

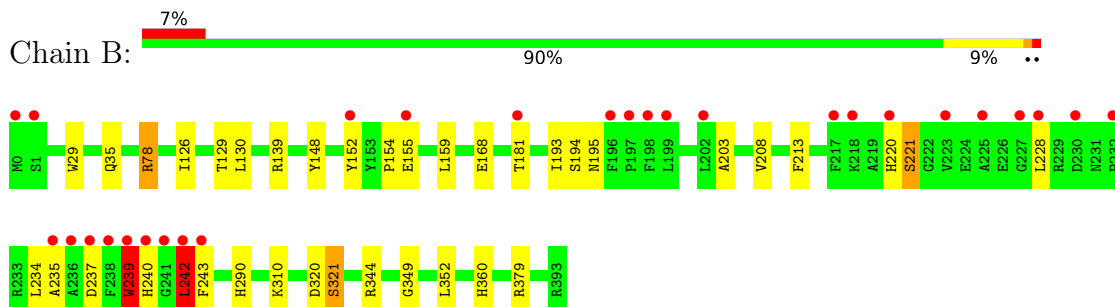
3 Residue-property plots [i](#)

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

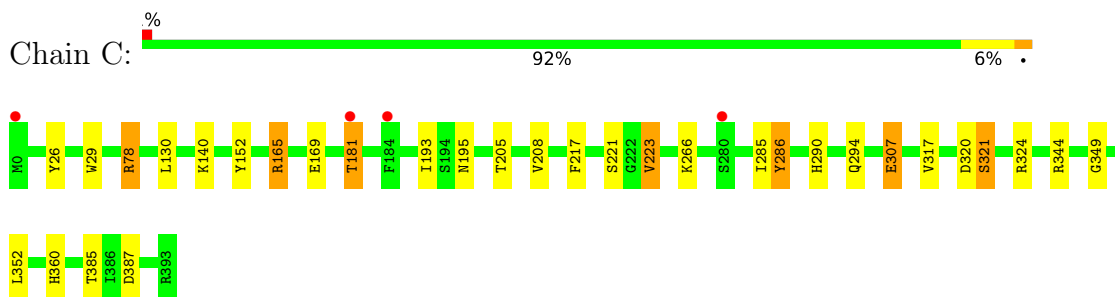
- Molecule 1: Lactate 2-monooxygenase



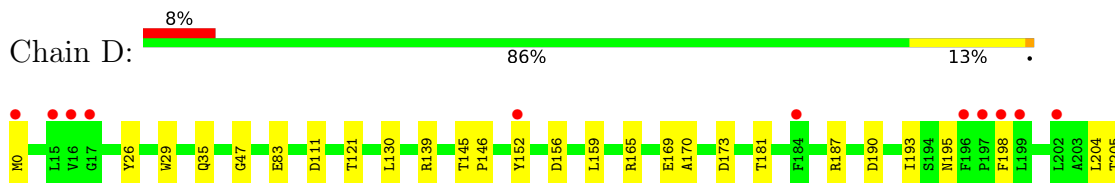
- Molecule 1: Lactate 2-monooxygenase

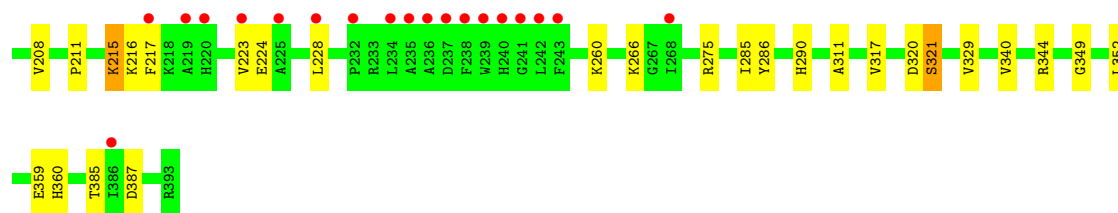


- Molecule 1: Lactate 2-monooxygenase

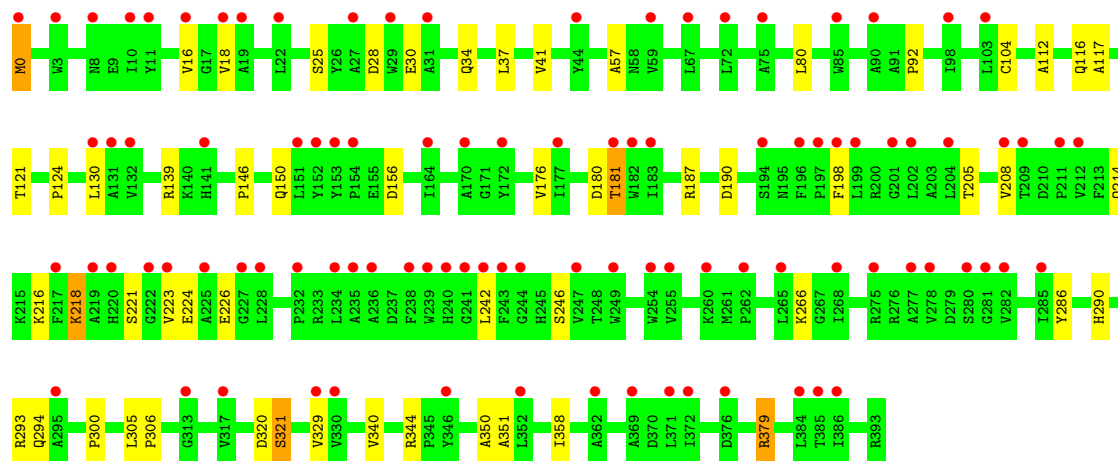
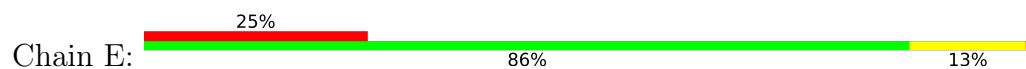


- Molecule 1: Lactate 2-monooxygenase

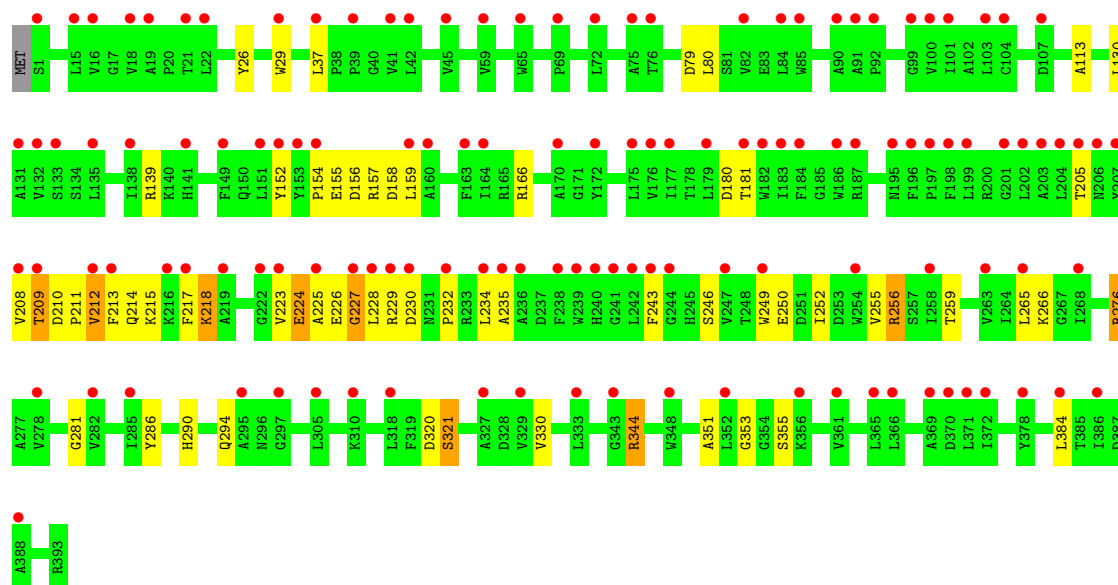
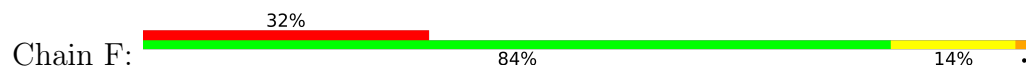




• Molecule 1: Lactate 2-monooxygenase



• Molecule 1: Lactate 2-monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	149.62Å 149.62Å 274.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.90 – 1.70 30.90 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.90-1.70) 99.9 (30.90-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 1.70Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.169 , 0.194 0.176 , 0.200	Depositor DCC
R_{free} test set	34003 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.8	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	0.97	EDS
Total number of atoms	20104	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, FMN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.84	0/3197	0.82	1/4353 (0.0%)
1	B	0.68	0/3286	0.73	1/4473 (0.0%)
1	C	0.60	0/3168	0.68	1/4311 (0.0%)
1	D	0.45	0/3164	0.55	0/4306
1	E	0.28	0/3140	0.40	0/4275
1	F	0.27	0/3134	0.43	0/4268
All	All	0.56	0/19089	0.62	3/25986 (0.0%)

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	B	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	ARG	CA-CB-CG	-6.75	100.59	114.10
1	A	1	SER	CA-C-O	-5.23	113.03	120.51
1	C	78	ARG	CA-CB-CG	-5.12	103.85	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	239[A]	TRP	Peptide

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Mol	Chain	Res	Type	Group
1	B	242[A]	LEU	Peptide

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	3080	0	3026	29	0
1	B	3166	0	3083	46	0
1	C	3066	0	3002	28	0
1	D	3062	0	2997	39	0
1	E	3043	0	2978	34	0
1	F	3037	0	2975	51	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	1	0
2	D	31	0	19	1	0
2	E	31	0	19	1	0
2	F	31	0	19	1	0
3	A	20	0	0	1	0
3	B	25	0	0	0	0
3	C	15	0	0	0	0
3	D	10	0	0	0	0
3	E	10	0	0	0	0
3	F	10	0	0	0	0
4	A	499	0	0	5	2
4	B	358	0	0	7	1
4	C	313	0	0	1	1
4	D	182	0	0	5	0
4	E	13	0	0	0	0
4	F	9	0	0	0	0
All	All	20104	0	18175	228	2

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 6.

All (228) 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:A:383:GLU:OE2	4:A:501:HOH:O	1.82	0.97
1:A:139:ARG:NH1	4:A:502:HOH:O	1.97	0.96
1:B:240[A]:HIS:O	1:B:243[A]:PHE:N	2.02	0.93
1:C:181[B]:THR:HG22	1:C:294:GLN:HG3	1.55	0.89
1:B:237[A]:ASP:O	1:B:239[A]:TRP:N	2.06	0.88
1:D:145:THR:O	4:D:501:HOH:O	1.93	0.85
1:D:139[A]:ARG:NH1	4:D:501:HOH:O	2.03	0.84
1:D:329:VAL:HG13	1:D:340[B]:VAL:HG21	1.64	0.79
1:B:155:GLU:H	1:B:242[A]:LEU:CD1	1.96	0.78
1:F:205:THR:O	1:F:209:THR:HG23	1.84	0.78
1:B:154:PRO:HB2	1:B:242[A]:LEU:HD11	1.66	0.78
1:F:256:ARG:NH2	1:F:281:GLY:O	2.17	0.78
1:E:181[B]:THR:HG22	1:E:294:GLN:HG3	1.64	0.77
1:F:225:ALA:HA	1:F:228:LEU:HB3	1.71	0.73
1:E:181[B]:THR:HG21	1:E:290:HIS:CE1	2.24	0.72
1:F:212:VAL:O	1:F:215:LYS:N	2.21	0.72
1:A:152:TYR:HE1	1:A:181[A]:THR:HG23	1.54	0.72
1:C:181[B]:THR:HG21	1:C:290:HIS:CE1	2.24	0.72
1:E:112:ALA:O	1:E:116:GLN:HG3	1.92	0.70
1:B:29[B]:TRP:CE3	1:B:352:LEU:HD12	2.25	0.70
1:B:168:GLU:OE1	4:B:501:HOH:O	2.09	0.70
1:A:279[A]:ASP:OD2	4:A:503:HOH:O	2.10	0.69
1:B:29[B]:TRP:HZ2	1:B:360:HIS:HD2	1.38	0.69
1:A:29[B]:TRP:CE3	1:A:352:LEU:HD12	2.29	0.67
1:F:181[B]:THR:HG22	1:F:294:GLN:HG3	1.76	0.67
1:B:155:GLU:N	1:B:242[A]:LEU:CD1	2.58	0.66
1:C:205:THR:HA	1:C:208[A]:VAL:HG22	1.79	0.65
1:B:234:LEU:HD11	4:B:648:HOH:O	1.97	0.64
1:F:226:GLU:O	1:F:230:ASP:N	2.29	0.64
1:A:29[B]:TRP:HZ2	1:A:360:HIS:HD2	1.46	0.64
1:C:152:TYR:HE1	1:C:181[A]:THR:HG23	1.63	0.63
1:F:208[B]:VAL:HG22	1:F:228:LEU:HG	1.79	0.63
1:A:35[A]:GLN:NE2	4:A:504:HOH:O	2.11	0.63
1:E:221:SER:OG	1:E:223:VAL:HG13	1.99	0.62
1:B:237[B]:ASP:N	1:B:237[B]:ASP:OD1	2.33	0.62
1:B:29[B]:TRP:CZ3	1:B:352:LEU:HD12	2.37	0.60
1:A:0:MET:HE2	1:A:0:MET:HA	1.82	0.60
1:B:155:GLU:N	1:B:242[A]:LEU:HD11	2.17	0.60
1:A:181[A]:THR:HG21	1:A:290:HIS:CE1	2.36	0.60
1:A:294:GLN:OE1	4:A:505[B]:HOH:O	2.17	0.60
1:D:266:LYS:HA	1:D:286:TYR:HB3	1.83	0.60
1:F:249:TRP:CH2	1:F:276:ARG:HG2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29[B]:TRP:HZ2	1:C:360:HIS:HD2	1.50	0.59
1:F:225:ALA:HA	1:F:228:LEU:CB	2.31	0.59
1:C:181[B]:THR:HG22	1:C:294:GLN:CG	2.32	0.58
1:C:181[B]:THR:CG2	1:C:294:GLN:HG3	2.30	0.58
1:A:205:THR:HA	1:A:208[A]:VAL:HG22	1.84	0.58
1:D:139[B]:ARG:HG2	1:D:170:ALA:O	2.04	0.58
1:B:193:ILE:HG13	1:B:195:ASN:HB2	1.85	0.58
1:D:211:PRO:O	1:D:215:LYS:HG2	2.03	0.58
1:E:266:LYS:HA	1:E:286:TYR:HB3	1.86	0.58
1:F:255:VAL:O	1:F:259:THR:HG22	2.04	0.57
1:B:155:GLU:H	1:B:242[A]:LEU:HD13	1.68	0.57
1:F:211:PRO:O	1:F:214:GLN:C	2.48	0.56
1:A:139:ARG:HG2	1:A:172:TYR:CZ	2.41	0.56
1:D:208:VAL:HG12	1:D:228:LEU:HG	1.86	0.56
1:F:226:GLU:C	1:F:228:LEU:N	2.64	0.55
1:C:165:ARG:O	1:C:169:GLU:HG3	2.06	0.55
1:D:29[A]:TRP:HZ2	1:D:360:HIS:HD2	1.53	0.55
1:E:180:ASP:OD1	1:E:181[B]:THR:HG23	2.06	0.55
1:A:152:TYR:CE1	1:A:181[A]:THR:HG23	2.39	0.55
1:A:29[B]:TRP:CZ3	1:A:352:LEU:HD12	2.43	0.54
1:B:239[A]:TRP:CE3	1:B:239[A]:TRP:HA	2.43	0.54
1:D:29[A]:TRP:CE3	1:D:352:LEU:HD12	2.43	0.54
1:D:139[A]:ARG:HG2	1:D:170:ALA:O	2.08	0.54
1:C:29[B]:TRP:CE3	1:C:352:LEU:HD12	2.43	0.54
1:D:130:LEU:HD13	1:D:198:PHE:CE1	2.43	0.54
1:E:130[B]:LEU:HD13	1:E:198:PHE:CZ	2.43	0.54
1:C:29[B]:TRP:CZ3	1:C:349:GLY:HA2	2.43	0.53
1:B:239[A]:TRP:HB3	1:B:242[A]:LEU:H	1.73	0.53
1:B:242[A]:LEU:HD12	1:B:242[A]:LEU:C	2.32	0.53
1:D:320:ASP:O	1:D:321:SER:HB2	2.08	0.53
1:B:155:GLU:HB2	1:B:242[A]:LEU:HD13	1.90	0.53
1:F:205:THR:HA	1:F:208[A]:VAL:HG22	1.91	0.53
1:A:29[B]:TRP:CZ2	1:A:360:HIS:HD2	2.27	0.53
1:E:187[B]:ARG:NE	1:E:190:ASP:OD2	2.37	0.53
1:C:152:TYR:CE1	1:C:181[A]:THR:HG23	2.43	0.53
1:B:154:PRO:CB	1:B:242[A]:LEU:HD11	2.36	0.52
1:F:266:LYS:HA	1:F:286:TYR:HB3	1.91	0.52
1:C:266:LYS:HA	1:C:286:TYR:HB3	1.90	0.52
1:B:193:ILE:O	1:B:194:SER:C	2.51	0.52
1:C:152:TYR:CE1	1:C:181[B]:THR:OG1	2.62	0.52
1:D:205:THR:HA	1:D:208:VAL:CG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:TYR:HE1	1:C:181[B]:THR:OG1	1.91	0.52
1:A:126:ILE:HG12	1:A:148:TYR:HB2	1.92	0.52
1:B:220:HIS:O	1:B:221:SER:HB3	2.10	0.52
1:F:227:GLY:CA	1:F:234:LEU:HD12	2.40	0.51
1:E:130[B]:LEU:HD13	1:E:198:PHE:CE1	2.45	0.51
1:F:26:TYR:HA	1:F:29:TRP:CE3	2.45	0.51
1:D:187[B]:ARG:NH2	1:D:190:ASP:OD2	2.41	0.51
1:F:159:LEU:CA	1:F:212:VAL:HG11	2.41	0.51
1:D:29[A]:TRP:CZ2	1:D:360:HIS:HD2	2.29	0.51
1:B:213:PHE:HE1	1:B:242[B]:LEU:HD21	1.77	0.50
1:B:239[A]:TRP:HA	1:B:239[A]:TRP:HE3	1.75	0.50
1:F:250:GLU:OE1	1:F:250:GLU:N	2.44	0.50
1:A:181[A]:THR:HG21	1:A:290:HIS:HE1	1.76	0.50
1:A:29[B]:TRP:CZ3	1:A:349:GLY:HA2	2.47	0.50
1:A:165:ARG:O	1:A:169:GLU:HG3	2.12	0.50
1:F:210:ASP:O	1:F:214:GLN:HB2	2.11	0.50
1:F:223:VAL:HG12	1:F:223:VAL:O	2.11	0.50
1:E:320:ASP:OD1	1:E:320:ASP:C	2.56	0.49
1:B:242[A]:LEU:HD12	1:B:242[A]:LEU:O	2.12	0.49
1:D:29[A]:TRP:HZ2	1:D:360:HIS:CD2	2.30	0.49
1:B:152:TYR:OH	4:B:502:HOH:O	2.19	0.49
1:B:220:HIS:O	1:B:221:SER:CB	2.61	0.49
1:E:350:ALA:HB2	1:E:358:ILE:HD11	1.93	0.49
1:F:218:LYS:HD3	1:F:224:GLU:HG3	1.95	0.49
1:B:193:ILE:HG13	1:B:195:ASN:CB	2.43	0.49
1:F:130[A]:LEU:HD21	1:F:243:PHE:HE1	1.77	0.49
1:F:218:LYS:NZ	1:F:224:GLU:OE1	2.45	0.49
1:E:205:THR:HA	1:E:208[A]:VAL:HG22	1.95	0.48
1:E:218:LYS:HD2	1:E:224:GLU:HA	1.94	0.48
1:E:329:VAL:HG13	1:E:340[A]:VAL:HG21	1.94	0.48
1:C:29[B]:TRP:CZ2	1:C:360:HIS:HD2	2.31	0.48
1:E:16:VAL:HG23	1:E:18:VAL:HG23	1.94	0.48
1:B:139:ARG:O	1:B:139:ARG:HD3	2.14	0.48
1:F:180:ASP:OD1	1:F:181[B]:THR:HG23	2.14	0.48
1:B:320:ASP:O	1:B:321:SER:HB2	2.14	0.48
1:C:307:GLU:HG3	4:C:566:HOH:O	2.13	0.48
1:F:208[A]:VAL:HG12	1:F:228:LEU:HG	1.95	0.48
1:F:223:VAL:HG11	1:F:234:LEU:HD13	1.96	0.47
1:A:157:ARG:HG2	1:A:254:TRP:CH2	2.49	0.47
1:F:212:VAL:HG12	1:F:213:PHE:N	2.28	0.47
1:B:228:LEU:HD13	1:B:235[B]:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181[B]:THR:CG2	1:C:290:HIS:CE1	2.98	0.47
1:C:385:THR:OG1	1:C:387:ASP:OD1	2.27	0.47
1:D:152:TYR:HE1	1:D:181:THR:HG1	1.62	0.47
1:F:227:GLY:O	1:F:234:LEU:HD12	2.15	0.47
1:B:237[B]:ASP:HB2	4:B:507:HOH:O	2.14	0.47
1:E:187[B]:ARG:NH2	1:E:190:ASP:OD2	2.48	0.47
1:F:227:GLY:HA3	1:F:234:LEU:HD12	1.97	0.47
1:F:228:LEU:O	1:F:232:PRO:HA	2.14	0.47
1:C:217:PHE:CE2	1:C:223:VAL:HG13	2.50	0.46
1:D:139[B]:ARG:NH1	4:D:501:HOH:O	2.47	0.46
1:B:129:THR:HB	1:B:152:TYR:HD2	1.80	0.46
1:D:320:ASP:OD1	1:D:320:ASP:C	2.59	0.46
1:D:111:ASP:OD1	1:D:111:ASP:N	2.48	0.46
1:F:320:ASP:O	1:F:321:SER:HB2	2.14	0.46
1:F:166:ARG:NH1	1:F:210:ASP:HB2	2.30	0.46
1:C:181[A]:THR:HG21	1:C:290:HIS:CE1	2.51	0.46
1:D:224:GLU:H	1:D:224:GLU:CD	2.24	0.46
1:A:139:ARG:HG2	1:A:172:TYR:CE2	2.51	0.45
1:E:218:LYS:HE3	1:E:224:GLU:CD	2.42	0.45
1:C:320:ASP:C	1:C:320:ASP:OD1	2.59	0.45
1:B:29[B]:TRP:CZ3	1:B:349:GLY:HA2	2.51	0.45
1:E:124:PRO:HB3	1:E:146:PRO:O	2.16	0.45
1:F:37:LEU:HD21	1:F:351:ALA:HB2	1.98	0.45
1:F:218:LYS:HZ2	1:F:224:GLU:CD	2.25	0.45
1:A:63:LYS:NZ	3:A:402:SO4:O3	2.45	0.45
1:D:121:THR:CG2	1:D:359:GLU:HG3	2.46	0.45
1:E:80:LEU:HB3	1:E:92:PRO:HD3	1.98	0.45
1:F:252:ILE:HD12	1:F:265:LEU:HD21	1.99	0.45
1:F:320:ASP:C	1:F:320:ASP:OD1	2.60	0.45
1:D:329:VAL:HG13	1:D:340[B]:VAL:CG2	2.39	0.45
1:D:139[A]:ARG:CZ	4:D:501:HOH:O	2.58	0.45
1:B:213:PHE:CE1	1:B:242[B]:LEU:HD21	2.52	0.44
1:D:156:ASP:OD2	1:D:216:LYS:HD3	2.17	0.44
1:D:193:ILE:HG13	1:D:195:ASN:HB2	1.99	0.44
1:B:35[A]:GLN:HG3	1:D:35:GLN:HG3	2.00	0.44
1:E:293:ARG:HD2	2:E:401:FMN:HM83	1.99	0.44
1:E:104:CYS:O	1:E:351:ALA:HA	2.17	0.44
1:D:385:THR:OG1	1:D:387:ASP:OD1	2.33	0.44
1:F:159:LEU:HB2	1:F:212:VAL:HG11	1.99	0.44
1:D:217:PHE:CE2	1:D:223:VAL:HB	2.53	0.44
1:E:37:LEU:HD22	1:E:41:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:ALA:O	1:E:121:THR:HG23	2.18	0.43
1:A:135:LEU:C	1:A:135:LEU:HD12	2.44	0.43
1:A:205:THR:HA	1:A:208[A]:VAL:CG2	2.48	0.43
1:F:226:GLU:C	1:F:228:LEU:H	2.26	0.43
1:D:152:TYR:HE1	1:D:181:THR:OG1	2.02	0.43
1:E:30:GLU:O	1:E:34:GLN:HG3	2.19	0.43
1:F:252:ILE:O	1:F:256:ARG:HG2	2.18	0.43
1:D:146:PRO:HA	1:D:173:ASP:OD2	2.18	0.43
1:F:159:LEU:HB2	1:F:212:VAL:CG1	2.49	0.43
1:F:212:VAL:C	1:F:215:LYS:H	2.21	0.43
1:D:156:ASP:OD2	1:D:216:LYS:CD	2.66	0.43
1:D:275:ARG:HG3	1:D:311:ALA:HB1	1.99	0.43
1:A:183:ILE:HG21	1:A:183:ILE:HD13	1.79	0.43
1:B:237[B]:ASP:HA	1:B:239[B]:TRP:HE1	1.83	0.43
1:E:156:ASP:OD2	1:E:216:LYS:HE3	2.18	0.42
1:F:154:PRO:C	1:F:156:ASP:H	2.27	0.42
1:A:23:PRO:HB2	1:A:29[A]:TRP:CD1	2.53	0.42
1:D:29[A]:TRP:CZ3	1:D:352:LEU:HD12	2.54	0.42
1:D:29[A]:TRP:CZ3	1:D:349:GLY:HA2	2.54	0.42
1:F:217:PHE:CE2	1:F:235:ALA:HB2	2.55	0.42
1:A:161:GLU:HG2	1:A:165:ARG:NH1	2.34	0.42
1:E:214:GLN:O	1:E:218:LYS:HB2	2.19	0.42
1:A:242:LEU:HD12	1:A:242:LEU:C	2.44	0.42
2:D:401:FMN:H9	2:D:401:FMN:O4'	2.20	0.42
1:F:79:ASP:C	1:F:80:LEU:HD12	2.45	0.42
1:F:113:ALA:HB1	1:F:355:SER:HB2	2.02	0.42
1:D:26:TYR:HA	1:D:29[B]:TRP:CE3	2.55	0.42
1:E:150:GLN:HA	1:E:176:VAL:O	2.19	0.42
1:E:320:ASP:O	1:E:321:SER:HB2	2.19	0.42
1:B:181[A]:THR:HG21	4:B:502:HOH:O	2.20	0.42
1:C:285:ILE:O	1:C:317:VAL:HA	2.20	0.42
1:B:78:ARG:HA	1:B:379:ARG:O	2.20	0.42
1:B:239[B]:TRP:CD1	1:B:239[B]:TRP:N	2.87	0.42
1:C:320:ASP:O	1:C:321:SER:HB2	2.19	0.42
1:E:25:SER:OG	1:E:28:ASP:OD2	2.37	0.42
1:E:242:LEU:C	1:E:242:LEU:HD12	2.45	0.42
1:B:181[A]:THR:CG2	1:B:290:HIS:CE1	3.03	0.41
1:B:310:LYS:NZ	4:B:526:HOH:O	2.52	0.41
1:E:57:ALA:HB1	1:E:300:PRO:HG3	2.03	0.41
1:B:242[B]:LEU:HD13	1:B:242[B]:LEU:N	2.35	0.41
1:C:26:TYR:HA	1:C:29[A]:TRP:CE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:159:LEU:N	1:F:212:VAL:HG11	2.36	0.41
1:C:26:TYR:CZ	1:C:324:ARG:HD2	2.55	0.41
1:B:181[B]:THR:HG21	4:B:502:HOH:O	2.19	0.41
1:F:181[B]:THR:HG21	1:F:290:HIS:CE1	2.55	0.41
1:B:320:ASP:OD1	1:B:320:ASP:C	2.64	0.41
1:E:0:MET:HE2	1:E:0:MET:HB3	1.96	0.41
1:B:126:ILE:HG12	1:B:148:TYR:HB2	2.03	0.41
1:B:130:LEU:HD21	1:B:243[A]:PHE:CZ	2.55	0.41
1:C:29[B]:TRP:HZ2	1:C:360:HIS:CD2	2.35	0.41
1:D:181:THR:HG21	1:D:290:HIS:CE1	2.56	0.41
1:E:305:LEU:HB3	1:E:306:PRO:HD3	2.02	0.41
1:E:379:ARG:HB2	1:E:379:ARG:CZ	2.51	0.41
1:F:330:VAL:HG13	1:F:384:LEU:HD21	2.03	0.41
1:F:344:ARG:HD3	2:F:401:FMN:C8M	2.52	0.41
1:A:320:ASP:C	1:A:320:ASP:OD1	2.64	0.40
1:D:285:ILE:O	1:D:317:VAL:HA	2.21	0.40
1:C:221:SER:OG	1:C:223:VAL:HG12	2.21	0.40
2:C:401:FMN:H9	2:C:401:FMN:O4'	2.22	0.40
1:D:47:GLY:HA3	4:D:617:HOH:O	2.21	0.40
1:C:193:ILE:HG13	1:C:195:ASN:HB2	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:584:HOH:O	4:B:604:HOH:O[7_555]	2.13	0.07
4:A:992:HOH:O	4:C:813:HOH:O[3_545]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	404/394 (102%)	392 (97%)	10 (2%)	2 (0%)	24	12
1	B	414/394 (105%)	397 (96%)	12 (3%)	5 (1%)	10	2
1	C	399/394 (101%)	389 (98%)	9 (2%)	1 (0%)	36	22
1	D	399/394 (101%)	388 (97%)	10 (2%)	1 (0%)	36	22
1	E	398/394 (101%)	384 (96%)	13 (3%)	1 (0%)	36	22
1	F	397/394 (101%)	373 (94%)	20 (5%)	4 (1%)	12	3
All	All	2411/2364 (102%)	2323 (96%)	74 (3%)	14 (1%)	21	9

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	B	321	SER
1	C	321	SER
1	D	321	SER
1	A	321	SER
1	B	221	SER
1	E	321	SER
1	F	227	GLY
1	B	203	ALA
1	B	239[A]	TRP
1	B	239[B]	TRP
1	F	224	GLU
1	F	321	SER
1	F	353	GLY

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	316/304 (104%)	308 (98%)	8 (2%)	42	24
1	B	322/304 (106%)	317 (98%)	5 (2%)	55	41
1	C	311/304 (102%)	301 (97%)	10 (3%)	34	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	311/304 (102%)	302 (97%)	9 (3%)	37	20
1	E	310/304 (102%)	301 (97%)	9 (3%)	37	20
1	F	309/304 (102%)	296 (96%)	13 (4%)	26	11
All	All	1879/1824 (103%)	1825 (97%)	54 (3%)	39	20

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MET
1	A	1	SER
1	A	9	GLU
1	A	83	GLU
1	A	139	ARG
1	A	181[A]	THR
1	A	181[B]	THR
1	A	344	ARG
1	B	159	LEU
1	B	208	VAL
1	B	242[A]	LEU
1	B	242[B]	LEU
1	B	344	ARG
1	C	78	ARG
1	C	130	LEU
1	C	140	LYS
1	C	165	ARG
1	C	181[A]	THR
1	C	181[B]	THR
1	C	223	VAL
1	C	286	TYR
1	C	307	GLU
1	C	344	ARG
1	D	0	MET
1	D	83	GLU
1	D	159	LEU
1	D	165	ARG
1	D	169	GLU
1	D	204	LEU
1	D	215	LYS
1	D	260	LYS
1	D	344	ARG
1	E	0	MET

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Mol	Chain	Res	Type
1	E	139	ARG
1	E	181[A]	THR
1	E	181[B]	THR
1	E	218	LYS
1	E	226	GLU
1	E	246	SER
1	E	344	ARG
1	E	379	ARG
1	F	139	ARG
1	F	152	TYR
1	F	155	GLU
1	F	157	ARG
1	F	158	ASP
1	F	209	THR
1	F	212	VAL
1	F	218	LYS
1	F	229	ARG
1	F	246	SER
1	F	256	ARG
1	F	276	ARG
1	F	344	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	195	ASN
1	D	34	GLN
1	D	231	ASN
1	E	109	HIS
1	E	240	HIS
1	F	290	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	404[A]	-	4,4,4	0.36	0	6,6,6	0.61	0
3	SO4	C	402	-	4,4,4	0.36	0	6,6,6	0.72	0
3	SO4	B	406[B]	-	4,4,4	0.48	0	6,6,6	0.36	0
3	SO4	B	403	-	4,4,4	0.26	0	6,6,6	0.37	0
3	SO4	E	403	-	4,4,4	0.24	0	6,6,6	0.23	0
3	SO4	D	402	-	4,4,4	0.38	0	6,6,6	0.70	0
3	SO4	A	402	-	4,4,4	0.53	0	6,6,6	0.80	0
3	SO4	F	403	-	4,4,4	0.28	0	6,6,6	0.27	0
2	FMN	E	401	-	33,33,33	1.59	5 (15%)	48,50,50	1.36	11 (22%)
2	FMN	F	401	-	33,33,33	1.57	4 (12%)	48,50,50	1.33	7 (14%)
3	SO4	F	402	-	4,4,4	0.23	0	6,6,6	0.20	0
2	FMN	D	401	-	33,33,33	1.65	5 (15%)	48,50,50	1.36	9 (18%)
2	FMN	A	401	-	33,33,33	1.94	7 (21%)	48,50,50	1.65	10 (20%)
3	SO4	D	403	-	4,4,4	0.49	0	6,6,6	0.39	0
3	SO4	C	404	-	4,4,4	0.28	0	6,6,6	0.20	0
3	SO4	C	403	-	4,4,4	0.21	0	6,6,6	0.99	0
3	SO4	A	405	-	4,4,4	0.36	0	6,6,6	0.17	0
2	FMN	B	401	-	33,33,33	1.93	7 (21%)	48,50,50	1.46	9 (18%)
3	SO4	B	404[A]	-	4,4,4	0.31	0	6,6,6	0.11	0
3	SO4	A	403	-	4,4,4	0.47	0	6,6,6	0.62	0
2	FMN	C	401	-	33,33,33	1.86	7 (21%)	48,50,50	1.25	6 (12%)
3	SO4	B	405	-	4,4,4	0.20	0	6,6,6	0.14	0
3	SO4	B	402	-	4,4,4	0.62	0	6,6,6	0.46	0
3	SO4	E	402	-	4,4,4	0.31	0	6,6,6	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	B	401	-	-	1/18/18/18	0/3/3/3
2	FMN	D	401	-	-	1/18/18/18	0/3/3/3
2	FMN	E	401	-	-	5/18/18/18	0/3/3/3
2	FMN	A	401	-	-	1/18/18/18	0/3/3/3
2	FMN	C	401	-	-	1/18/18/18	0/3/3/3
2	FMN	F	401	-	-	5/18/18/18	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	FMN	C9A-C5A	5.79	1.50	1.41
2	F	401	FMN	C9A-C5A	5.75	1.50	1.41
2	E	401	FMN	C9A-C5A	5.67	1.50	1.41
2	D	401	FMN	C9A-C5A	5.19	1.49	1.41
2	A	401	FMN	C5'-C4'	4.95	1.58	1.51
2	C	401	FMN	C4A-N5	4.81	1.41	1.30
2	B	401	FMN	C5'-C4'	4.47	1.57	1.51
2	A	401	FMN	C4-N3	-4.06	1.31	1.38
2	B	401	FMN	C4A-N5	3.90	1.39	1.30
2	F	401	FMN	C8-C7	3.84	1.50	1.40
2	D	401	FMN	C4A-N5	3.79	1.38	1.30
2	A	401	FMN	C9A-C5A	3.71	1.47	1.41
2	A	401	FMN	C8-C7	3.65	1.49	1.40
2	C	401	FMN	O2-C2	3.63	1.31	1.24
2	B	401	FMN	O4-C4	3.50	1.30	1.23
2	C	401	FMN	C9A-C5A	3.45	1.46	1.41
2	E	401	FMN	C8-C7	3.37	1.49	1.40
2	C	401	FMN	C9A-N10	3.28	1.46	1.41
2	B	401	FMN	C5A-N5	-3.18	1.33	1.39
2	A	401	FMN	C10-N10	3.14	1.44	1.37
2	C	401	FMN	C10-N1	3.09	1.39	1.33
2	A	401	FMN	C9A-N10	-2.68	1.36	1.41
2	D	401	FMN	C9A-N10	2.62	1.45	1.41
2	A	401	FMN	O4-C4	2.55	1.28	1.23
2	C	401	FMN	C2-N3	-2.38	1.33	1.39
2	D	401	FMN	C8-C7	2.37	1.46	1.40
2	B	401	FMN	C8-C7	2.33	1.46	1.40
2	E	401	FMN	C4A-N5	2.27	1.35	1.30
2	D	401	FMN	O2-C2	2.23	1.28	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	FMN	C4-N3	-2.22	1.34	1.38
2	F	401	FMN	C4A-N5	2.17	1.35	1.30
2	B	401	FMN	C10-N1	2.17	1.37	1.33
2	C	401	FMN	C8-C7	2.16	1.46	1.40
2	E	401	FMN	C10-N10	2.14	1.42	1.37
2	F	401	FMN	C10-N10	2.03	1.41	1.37

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	FMN	O4-C4-C4A	-3.82	116.45	126.53
2	B	401	FMN	C4-C4A-N5	3.58	123.16	118.21
2	A	401	FMN	C9A-C5A-N5	-3.58	118.66	122.45
2	A	401	FMN	C5A-C9A-N10	3.55	121.18	117.97
2	A	401	FMN	C4-C4A-N5	3.28	122.73	118.21
2	D	401	FMN	C4-C4A-N5	3.20	122.62	118.21
2	A	401	FMN	C4A-C4-N3	2.98	120.84	113.25
2	C	401	FMN	O2-C2-N1	-2.90	116.99	121.80
2	A	401	FMN	C9-C9A-N10	-2.88	117.99	121.85
2	E	401	FMN	C4A-C10-N1	-2.80	117.73	124.59
2	B	401	FMN	C4A-C4-N3	2.78	120.33	113.25
2	F	401	FMN	C4-C4A-N5	2.77	122.03	118.21
2	B	401	FMN	O2-C2-N1	-2.74	117.25	121.80
2	A	401	FMN	O3P-P-O5'	-2.74	99.53	106.67
2	F	401	FMN	C9A-N10-C10	-2.63	116.74	120.75
2	D	401	FMN	C4A-C10-N10	2.61	120.22	116.48
2	C	401	FMN	O5'-P-O1P	-2.60	99.41	106.44
2	D	401	FMN	O5'-P-O1P	-2.56	99.52	106.44
2	E	401	FMN	C4'-C3'-C2'	-2.54	109.34	113.57
2	B	401	FMN	O4-C4-C4A	-2.53	119.86	126.53
2	A	401	FMN	O2-C2-N1	-2.50	117.64	121.80
2	F	401	FMN	C4A-C10-N1	-2.49	118.48	124.59
2	B	401	FMN	O3'-C3'-C4'	-2.48	103.30	108.93
2	B	401	FMN	C10-N1-C2	2.47	122.20	116.85
2	D	401	FMN	O2-C2-N1	-2.47	117.70	121.80
2	C	401	FMN	C9A-N10-C10	-2.45	117.01	120.75
2	E	401	FMN	C4-C4A-N5	2.44	121.58	118.21
2	D	401	FMN	O3P-P-O2P	2.41	116.86	107.80
2	B	401	FMN	O2'-C2'-C3'	-2.41	103.60	109.25
2	C	401	FMN	C4-C4A-N5	2.34	121.44	118.21
2	E	401	FMN	C10-N1-C2	2.31	121.85	116.85
2	D	401	FMN	C4A-C4-N3	2.23	118.92	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	FMN	C9A-N10-C10	-2.20	117.39	120.75
2	F	401	FMN	C10-N1-C2	2.20	121.62	116.85
2	E	401	FMN	O4-C4-C4A	-2.18	120.77	126.53
2	E	401	FMN	C9A-N10-C10	-2.17	117.44	120.75
2	E	401	FMN	O3P-P-O2P	2.16	115.89	107.80
2	F	401	FMN	O2P-P-O5'	-2.15	101.06	106.67
2	E	401	FMN	C4A-C4-N3	2.11	118.61	113.25
2	B	401	FMN	C8M-C8-C9	2.10	123.28	119.57
2	F	401	FMN	O5'-P-O1P	-2.10	100.76	106.44
2	A	401	FMN	C1'-N10-C9A	2.10	124.71	120.63
2	C	401	FMN	C4A-C4-N3	2.08	118.56	113.25
2	E	401	FMN	C4-N3-C2	-2.08	121.95	125.64
2	E	401	FMN	C4A-C10-N10	2.07	119.44	116.48
2	D	401	FMN	C10-N1-C2	2.06	121.31	116.85
2	F	401	FMN	O3P-P-O2P	2.06	115.52	107.80
2	B	401	FMN	C4A-C10-N1	-2.06	119.54	124.59
2	D	401	FMN	O4-C4-C4A	-2.04	121.15	126.53
2	E	401	FMN	O5'-P-O1P	-2.03	100.95	106.44
2	A	401	FMN	O2'-C2'-C3'	-2.02	104.53	109.25
2	C	401	FMN	C4A-C10-N10	2.01	119.36	116.48

There are no chirality outliers.

All (14) torsion outliers are listed below:

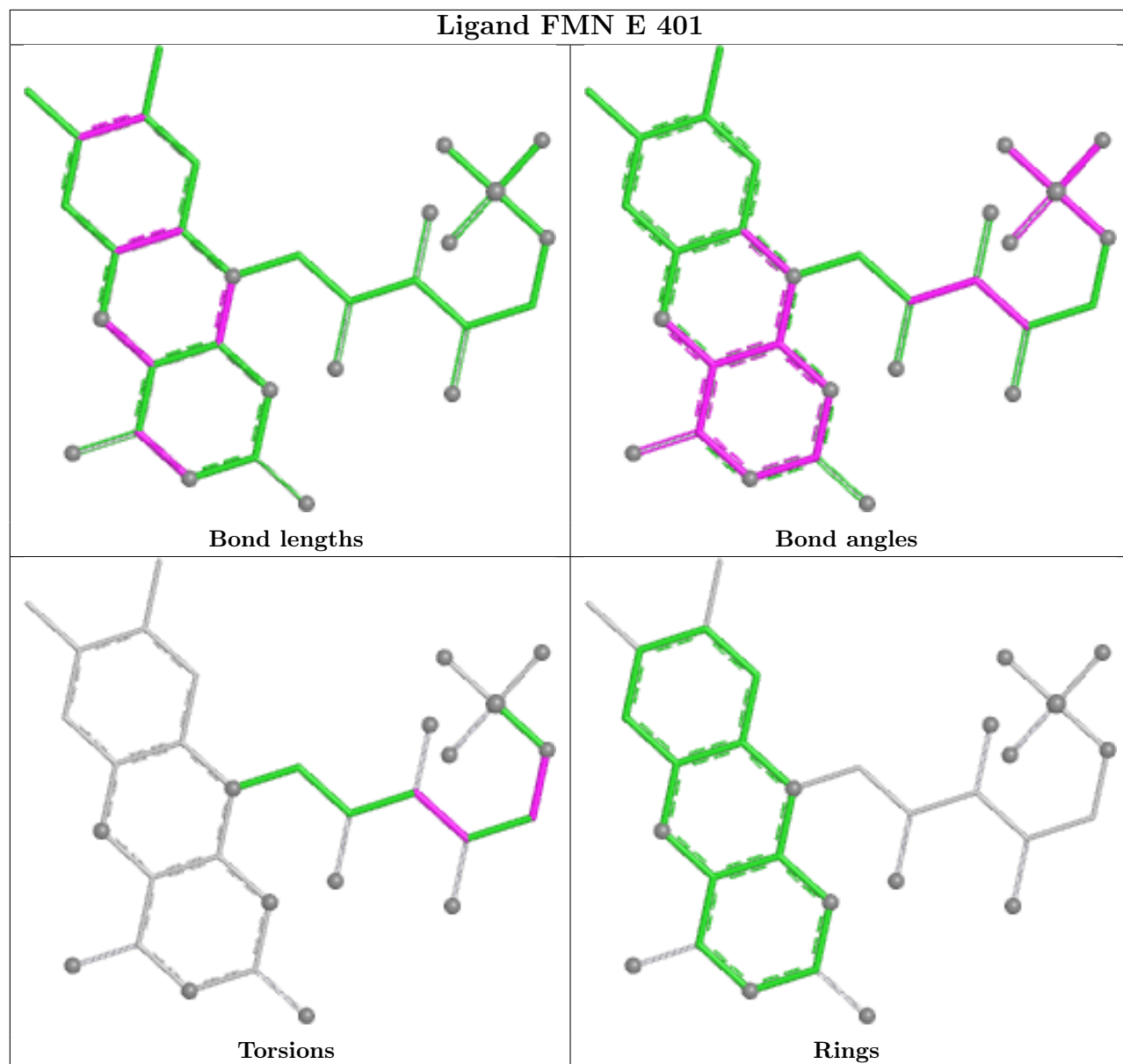
Mol	Chain	Res	Type	Atoms
2	E	401	FMN	C2'-C3'-C4'-O4'
2	F	401	FMN	C2'-C3'-C4'-O4'
2	F	401	FMN	C2'-C3'-C4'-C5'
2	F	401	FMN	O3'-C3'-C4'-C5'
2	B	401	FMN	C4'-C5'-O5'-P
2	C	401	FMN	C4'-C5'-O5'-P
2	E	401	FMN	C4'-C5'-O5'-P
2	E	401	FMN	C2'-C3'-C4'-C5'
2	A	401	FMN	C4'-C5'-O5'-P
2	D	401	FMN	C4'-C5'-O5'-P
2	F	401	FMN	C4'-C5'-O5'-P
2	F	401	FMN	O3'-C3'-C4'-O4'
2	E	401	FMN	O3'-C3'-C4'-C5'
2	E	401	FMN	O3'-C3'-C4'-O4'

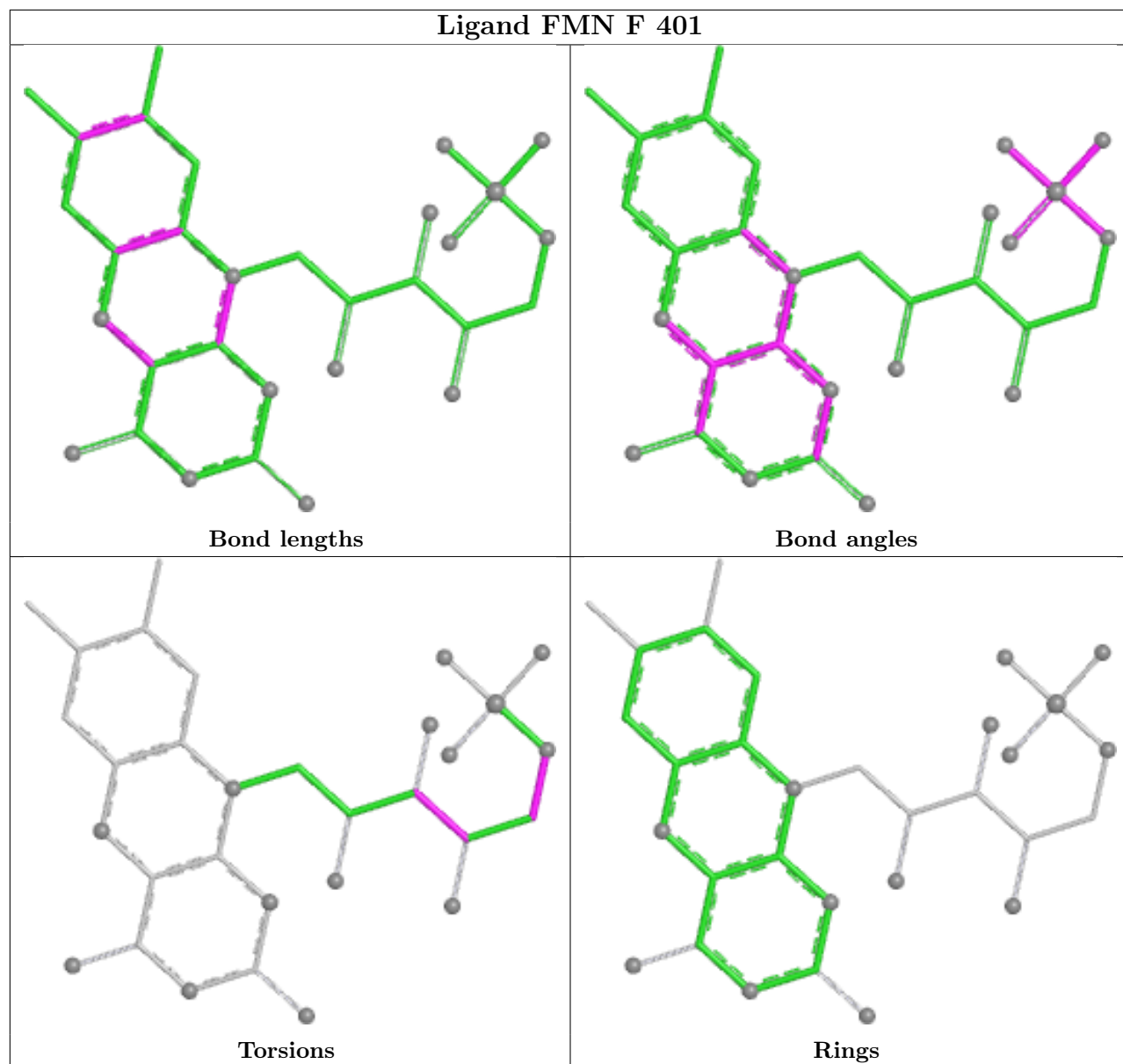
There are no ring outliers.

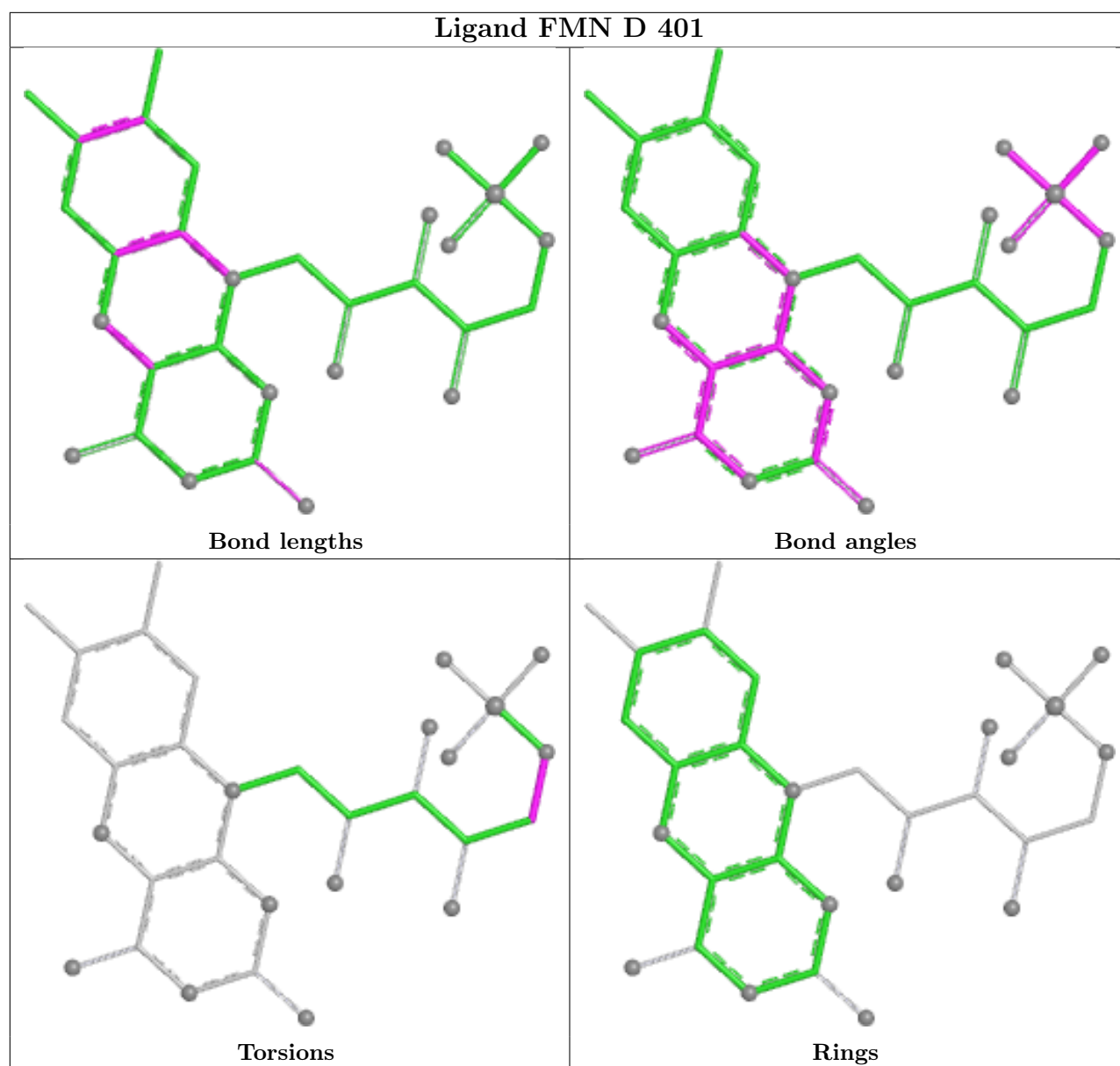
5 monomers are involved in 5 short contacts:

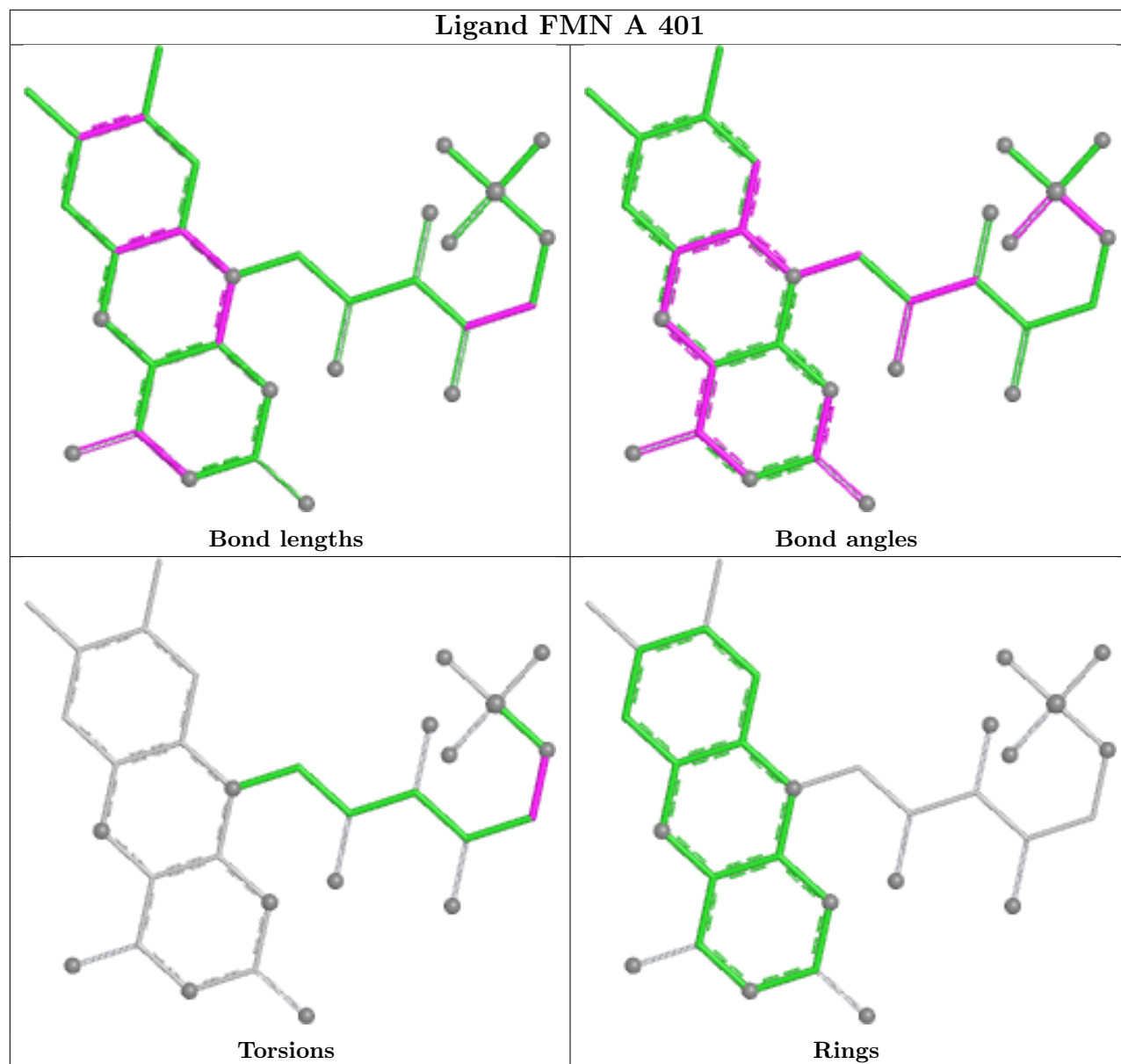
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	SO4	1	0
2	E	401	FMN	1	0
2	F	401	FMN	1	0
2	D	401	FMN	1	0
2	C	401	FMN	1	0

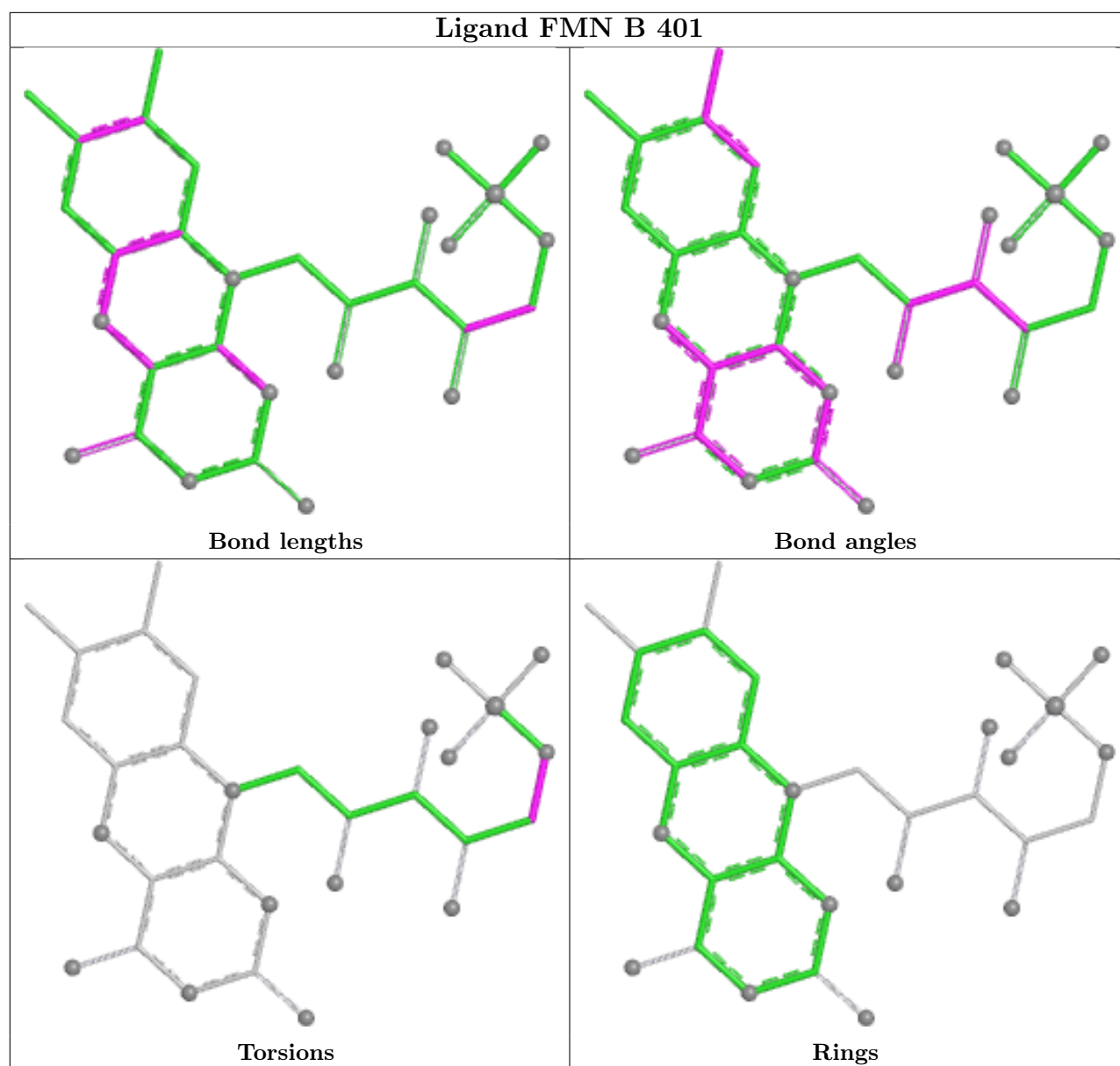
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

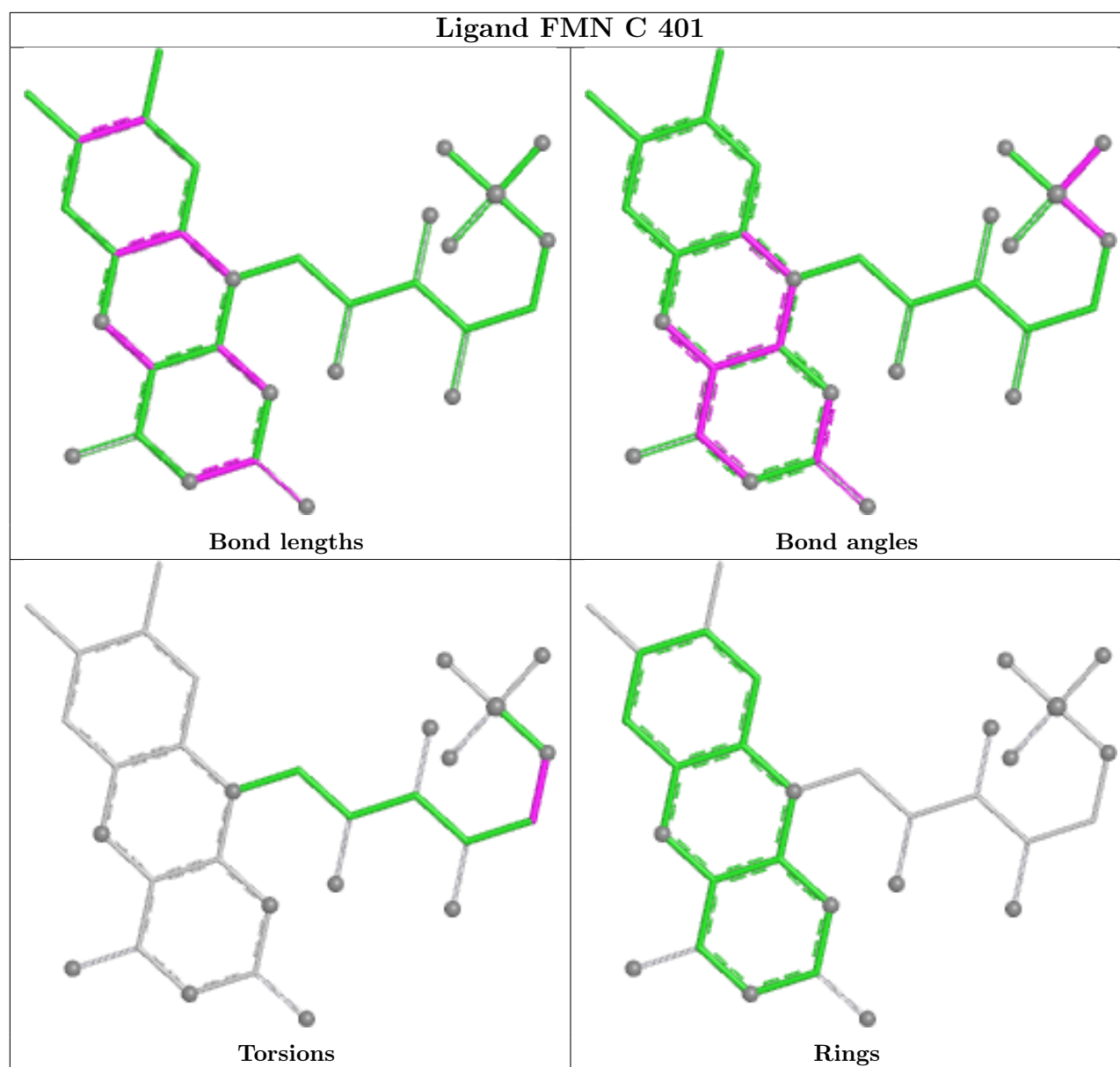












5.7 Other polymers [i](#)

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	394/394 (100%)	-0.43	2 (0%) 87 89	14, 29, 49, 77	12 (3%)
1	B	394/394 (100%)	0.17	28 (7%) 22 24	17, 37, 80, 131	22 (5%)
1	C	394/394 (100%)	-0.01	4 (1%) 79 82	17, 43, 70, 100	7 (1%)
1	D	394/394 (100%)	0.62	30 (7%) 20 21	28, 62, 103, 160	7 (1%)
1	E	394/394 (100%)	1.49	97 (24%) 2 2	42, 82, 127, 152	394 (100%)
1	F	393/394 (99%)	1.62	128 (32%) 1 1	46, 90, 135, 163	393 (100%)
All	All	2363/2364 (99%)	0.58	289 (12%) 8 8	14, 56, 111, 163	835 (35%)

All (289) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	239[A]	TRP	12.3
1	D	239	TRP	7.1
1	F	223	VAL	6.0
1	B	240[A]	HIS	5.9
1	B	238[A]	PHE	5.6
1	A	0	MET	5.3
1	B	0	MET	5.2
1	B	243[A]	PHE	4.9
1	F	132	VAL	4.9
1	B	235[A]	ALA	4.8
1	F	228	LEU	4.7
1	E	239	TRP	4.7
1	C	0	MET	4.7
1	D	238	PHE	4.6
1	F	242	LEU	4.6
1	B	198	PHE	4.6
1	F	239	TRP	4.5
1	E	223	VAL	4.4
1	D	235	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	242	LEU	4.3
1	D	198	PHE	4.3
1	B	202	LEU	4.3
1	F	184	PHE	4.3
1	B	236[A]	ALA	4.2
1	D	236	ALA	4.2
1	D	232	PRO	4.1
1	B	242[A]	LEU	4.1
1	F	234	LEU	4.1
1	D	0	MET	4.0
1	E	236	ALA	4.0
1	E	225	ALA	4.0
1	D	199	LEU	3.9
1	E	29	TRP	3.9
1	F	243	PHE	3.9
1	F	202	LEU	3.9
1	E	198	PHE	3.9
1	F	386	ILE	3.8
1	F	16	VAL	3.8
1	E	202	LEU	3.8
1	E	386	ILE	3.7
1	F	149	PHE	3.7
1	F	29	TRP	3.7
1	F	164	ILE	3.6
1	D	225	ALA	3.6
1	E	234	LEU	3.6
1	B	237[A]	ASP	3.6
1	F	213	PHE	3.5
1	E	242	LEU	3.5
1	F	212	VAL	3.5
1	F	152	TYR	3.5
1	F	238	PHE	3.4
1	E	228	LEU	3.4
1	E	132	VAL	3.4
1	E	131	ALA	3.4
1	F	247	VAL	3.4
1	E	235	ALA	3.3
1	F	131	ALA	3.3
1	D	240	HIS	3.3
1	F	82	VAL	3.3
1	F	90	ALA	3.3
1	F	101	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	258	ILE	3.3
1	B	197	PRO	3.3
1	F	232	PRO	3.3
1	F	352	LEU	3.3
1	E	182	TRP	3.2
1	F	198	PHE	3.2
1	F	18	VAL	3.2
1	B	228	LEU	3.2
1	F	236	ALA	3.2
1	E	194	SER	3.2
1	F	69	PRO	3.2
1	E	0	MET	3.2
1	F	99	GLY	3.2
1	E	11	TYR	3.1
1	F	197	PRO	3.1
1	E	208[A]	VAL	3.1
1	F	183	ILE	3.1
1	E	384	LEU	3.1
1	F	196	PHE	3.1
1	B	223	VAL	3.1
1	F	208[A]	VAL	3.1
1	F	153	TYR	3.1
1	E	183	ILE	3.1
1	E	219	ALA	3.1
1	F	203	ALA	3.1
1	F	163	PHE	3.1
1	E	244	GLY	3.0
1	F	207	TYR	3.0
1	B	217	PHE	3.0
1	E	16	VAL	3.0
1	F	278	VAL	3.0
1	F	282	VAL	3.0
1	F	225	ALA	3.0
1	D	228	LEU	3.0
1	E	151	LEU	3.0
1	E	199	LEU	3.0
1	E	243	PHE	2.9
1	E	330	VAL	2.9
1	E	241	GLY	2.9
1	D	197	PRO	2.9
1	A	1	SER	2.9
1	E	238	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	59	VAL	2.9
1	E	255	VAL	2.9
1	E	75	ALA	2.9
1	B	225	ALA	2.8
1	B	241[A]	GLY	2.8
1	B	199	LEU	2.8
1	F	103	LEU	2.8
1	F	187[A]	ARG	2.8
1	F	333	LEU	2.8
1	F	366	LEU	2.8
1	D	196	PHE	2.8
1	E	247	VAL	2.8
1	D	202	LEU	2.8
1	D	220	HIS	2.8
1	F	19	ALA	2.7
1	F	186	TRP	2.7
1	E	172	TYR	2.7
1	F	285	ILE	2.7
1	E	232	PRO	2.7
1	E	19	ALA	2.7
1	D	243	PHE	2.7
1	F	249	TRP	2.7
1	D	234	LEU	2.7
1	F	181[A]	THR	2.7
1	F	216	LYS	2.7
1	D	237	ASP	2.7
1	F	39	PRO	2.6
1	C	184	PHE	2.6
1	F	227	GLY	2.6
1	F	159	LEU	2.6
1	F	199	LEU	2.6
1	F	100	VAL	2.6
1	F	263	VAL	2.6
1	E	275	ARG	2.6
1	E	295	ALA	2.6
1	E	196	PHE	2.6
1	E	217	PHE	2.6
1	F	254	TRP	2.6
1	F	235	ALA	2.6
1	B	232	PRO	2.6
1	F	15	LEU	2.6
1	E	152	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	346	TYR	2.6
1	F	91	ALA	2.6
1	F	369	ALA	2.6
1	F	388	ALA	2.6
1	F	85	TRP	2.6
1	F	222	GLY	2.5
1	F	209	THR	2.5
1	F	22	LEU	2.5
1	E	212	VAL	2.5
1	E	278	VAL	2.5
1	F	217	PHE	2.5
1	E	265	LEU	2.5
1	E	352	LEU	2.5
1	D	16	VAL	2.5
1	F	59	VAL	2.5
1	F	160	ALA	2.5
1	E	376	ASP	2.5
1	F	384	LEU	2.5
1	E	90	ALA	2.5
1	E	10	ILE	2.5
1	E	317	VAL	2.5
1	E	329	VAL	2.5
1	F	205	THR	2.5
1	E	103	LEU	2.4
1	D	241	GLY	2.4
1	F	219	ALA	2.4
1	B	152	TYR	2.4
1	E	153	TYR	2.4
1	E	385	THR	2.4
1	F	1	SER	2.4
1	F	329	VAL	2.4
1	E	211	PRO	2.4
1	F	84	LEU	2.4
1	F	179	LEU	2.4
1	F	371	LEU	2.4
1	E	31	ALA	2.4
1	D	223	VAL	2.4
1	D	15	LEU	2.4
1	F	21	THR	2.4
1	E	249	TRP	2.4
1	F	370	ASP	2.4
1	E	154	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	217	PHE	2.3
1	E	3	TRP	2.3
1	E	268	ILE	2.3
1	E	281	GLY	2.3
1	F	297	GLY	2.3
1	E	260	LYS	2.3
1	D	219	ALA	2.3
1	F	295	ALA	2.3
1	F	327	ALA	2.3
1	E	67	LEU	2.3
1	F	135	LEU	2.3
1	F	151	LEU	2.3
1	F	172	TYR	2.3
1	D	268	ILE	2.3
1	F	138	ILE	2.3
1	C	280	SER	2.3
1	E	254	TRP	2.3
1	F	182	TRP	2.3
1	B	220	HIS	2.3
1	E	240	HIS	2.3
1	F	72	LEU	2.3
1	B	155	GLU	2.3
1	F	244	GLY	2.3
1	F	45	VAL	2.3
1	E	220	HIS	2.2
1	F	92	PRO	2.2
1	C	181[A]	THR	2.2
1	E	209	THR	2.2
1	F	76	THR	2.2
1	F	204[A]	LEU	2.2
1	F	318	LEU	2.2
1	B	227	GLY	2.2
1	D	152	TYR	2.2
1	E	44	TYR	2.2
1	E	98	ILE	2.2
1	E	18	VAL	2.2
1	F	41	VAL	2.2
1	F	348	TRP	2.2
1	F	75	ALA	2.2
1	F	170	ALA	2.2
1	F	133	SER	2.2
1	E	130[A]	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	241	GLY	2.2
1	B	196	PHE	2.2
1	D	184	PHE	2.2
1	F	240	HIS	2.2
1	F	154	PRO	2.2
1	D	17	GLY	2.2
1	E	22	LEU	2.2
1	E	227	GLY	2.2
1	E	371	LEU	2.2
1	F	365	LEU	2.2
1	F	177	ILE	2.2
1	F	372	ILE	2.2
1	E	181[A]	THR	2.2
1	B	1	SER	2.2
1	F	361	VAL	2.1
1	E	313	GLY	2.1
1	F	201	GLY	2.1
1	E	72	LEU	2.1
1	F	265	LEU	2.1
1	B	218	LYS	2.1
1	E	197	PRO	2.1
1	E	262	PRO	2.1
1	E	164	ILE	2.1
1	E	362	ALA	2.1
1	F	206	ASN	2.1
1	E	204	LEU	2.1
1	F	42	LEU	2.1
1	F	305	LEU	2.1
1	B	230	ASP	2.1
1	F	65	TRP	2.1
1	F	107	ASP	2.1
1	B	181[A]	THR	2.1
1	E	285	ILE	2.1
1	F	268	ILE	2.1
1	E	141	HIS	2.1
1	E	27	ALA	2.1
1	E	201	GLY	2.1
1	E	222	GLY	2.1
1	E	369	ALA	2.1
1	F	310	LYS	2.1
1	F	343	GLY	2.1
1	E	282	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	176	VAL	2.1
1	F	37	LEU	2.1
1	E	85	TRP	2.1
1	F	141	HIS	2.1
1	E	177	ILE	2.1
1	E	170	ALA	2.0
1	F	195	ASN	2.0
1	F	230	ASP	2.0
1	F	175	LEU	2.0
1	E	8	ASN	2.0
1	D	386	ILE	2.0
1	E	372	ILE	2.0
1	F	229	ARG	2.0
1	F	378	TYR	2.0
1	E	277	ALA	2.0
1	E	280[A]	SER	2.0
1	F	104	CYS	2.0
1	F	356	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	F	402	5/5	0.76	0.12	88,89,89,90	5
3	SO4	B	404[A]	5/5	0.77	0.13	67,67,68,70	5
2	FMN	F	401	31/31	0.77	0.12	74,79,82,82	31
3	SO4	E	403	5/5	0.80	0.11	94,95,95,96	5
2	FMN	E	401	31/31	0.81	0.12	74,78,81,81	31

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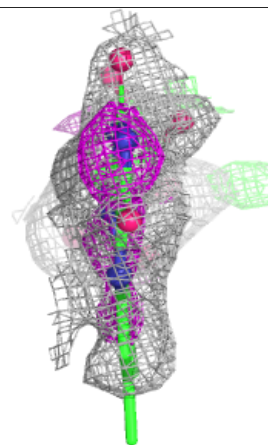
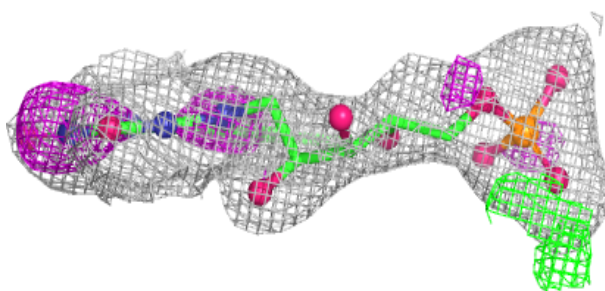
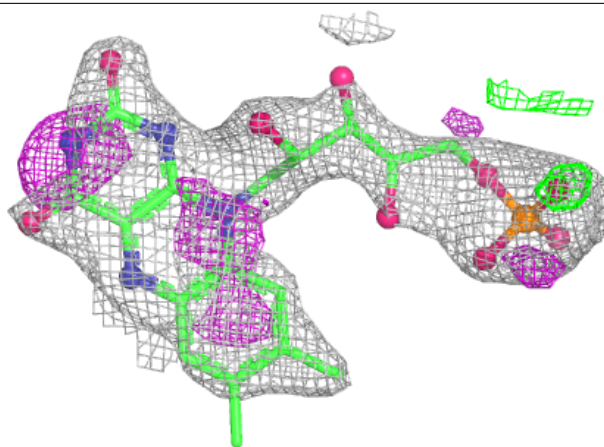
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	405	5/5	0.81	0.10	99,99,101,104	0
3	SO4	A	404[A]	5/5	0.82	0.22	50,56,58,59	5
3	SO4	B	406[B]	5/5	0.84	0.19	50,56,56,59	5
3	SO4	C	404	5/5	0.86	0.11	66,66,67,68	5
3	SO4	A	405	5/5	0.89	0.11	63,64,64,65	5
3	SO4	E	402	5/5	0.89	0.08	98,98,99,99	0
3	SO4	F	403	5/5	0.89	0.08	72,72,74,74	5
3	SO4	D	403	5/5	0.94	0.10	64,64,69,71	0
3	SO4	D	402	5/5	0.96	0.06	51,51,55,56	0
2	FMN	C	401	31/31	0.97	0.07	29,33,37,39	0
2	FMN	D	401	31/31	0.97	0.07	39,46,51,52	0
2	FMN	A	401	31/31	0.98	0.05	19,23,26,30	0
3	SO4	C	402	5/5	0.98	0.05	39,44,46,49	0
2	FMN	B	401	31/31	0.98	0.05	23,29,33,36	0
3	SO4	B	402	5/5	0.99	0.04	38,39,43,43	0
3	SO4	B	403	5/5	0.99	0.04	38,40,44,45	0
3	SO4	C	403	5/5	0.99	0.04	36,42,43,45	0
3	SO4	A	402	5/5	0.99	0.04	30,34,35,37	0
3	SO4	A	403	5/5	0.99	0.04	35,35,39,39	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.

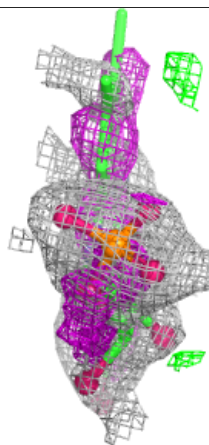
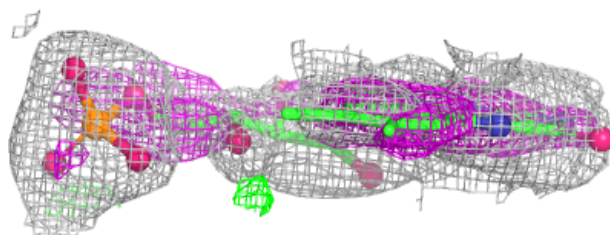
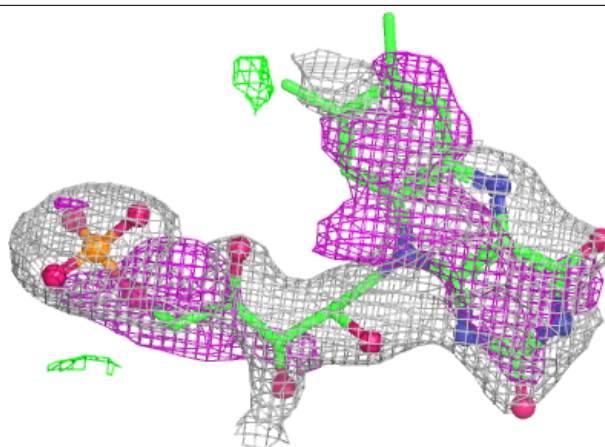
Electron density around FMN F 401:

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



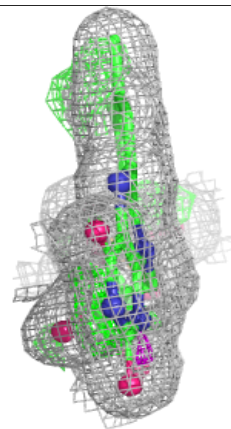
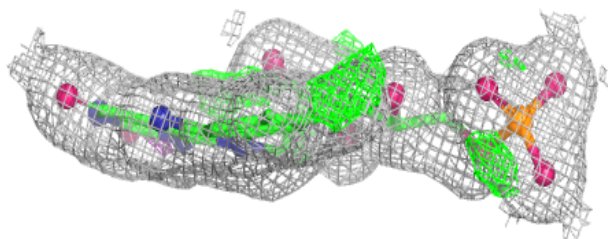
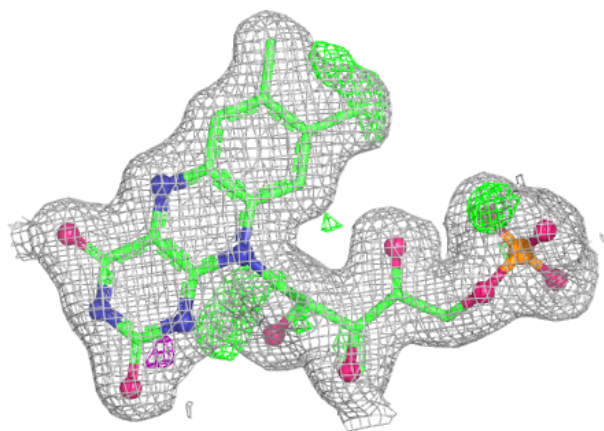
Electron density around FMN E 401:

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



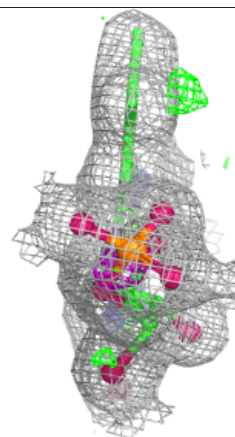
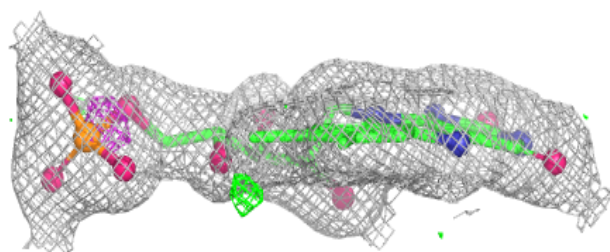
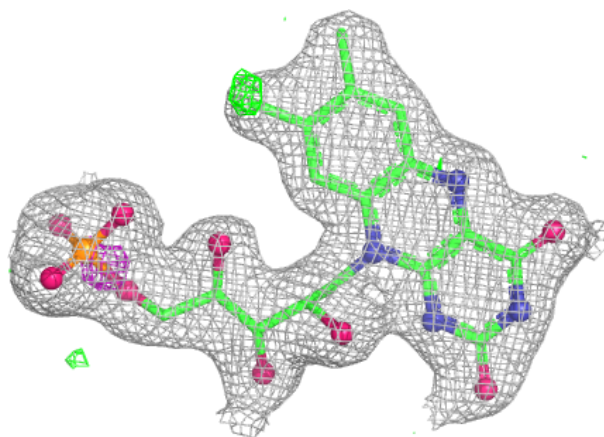
Electron density around FMN C 401:

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and green (positive)



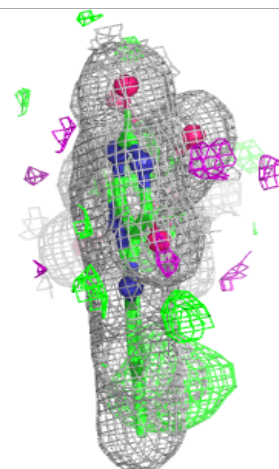
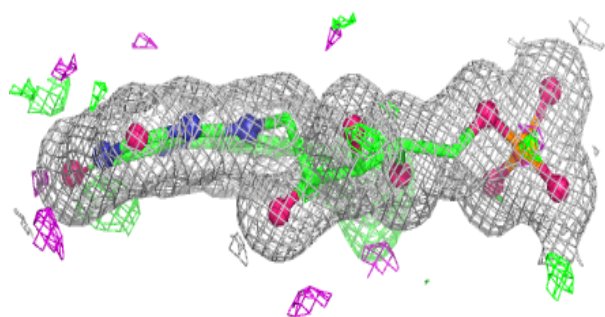
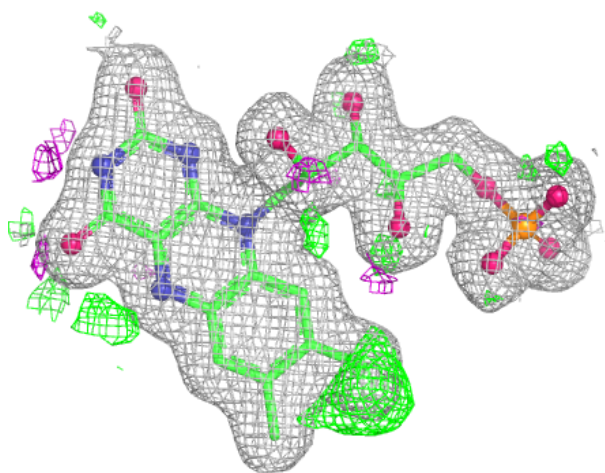
Electron density around FMN D 401:

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and green (positive)



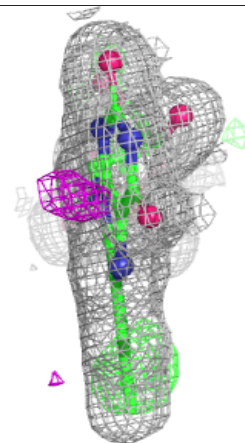
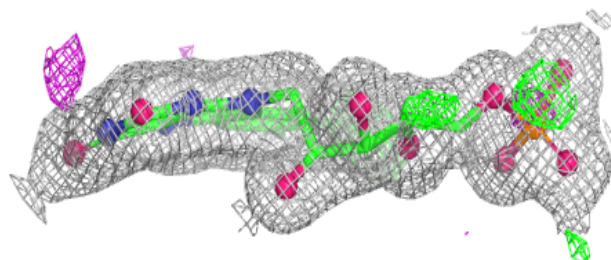
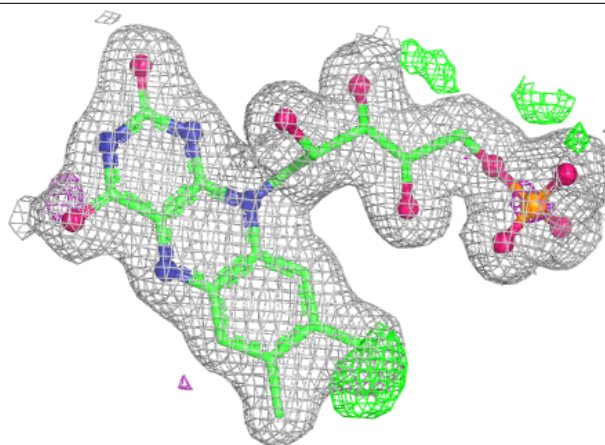
Electron density around FMN A 401:

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



Electron density around FMN B 401:

$2mF_o-DF_c$ (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.