Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 07:57 AM EDT

PDB ID	:	6DVI
Title	:	Wild-type Lactate Monooxygenase from Mycobacterium smegmatis
Authors	:	Kean, K.M.; Karplus, P.A.
Deposited on	:	2018-06-23
Resolution	:	2.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

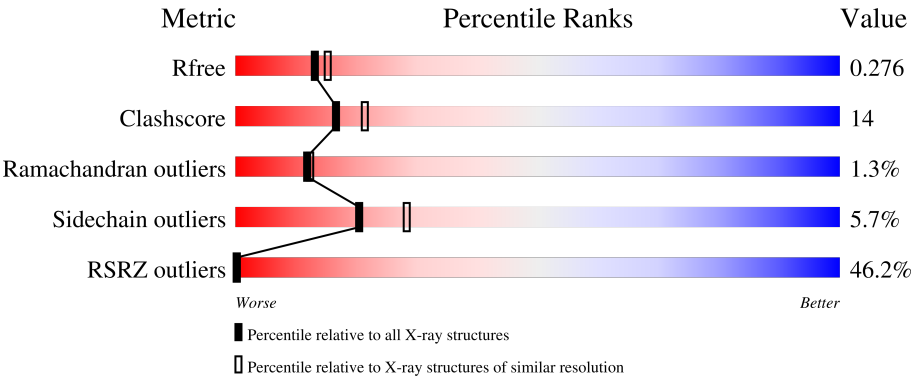
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	7% 86% 13%
1	B	394	20% 68% 26% 5%
1	C	394	4% 81% 18%
1	D	394	53% 46% 33% 5% 14%
1	E	394	92% 73% 25%

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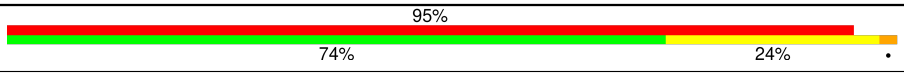
Mol	Chain	Length	Quality of chain
1	F	394	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FMN	E	401	-	-	-	X
3	SO4	B	404	-	-	-	X
3	SO4	F	402	-	-	-	X

2 Entry composition

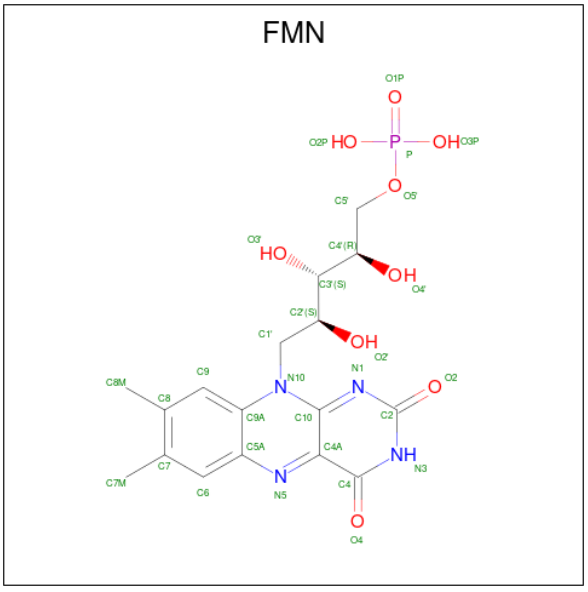
There are 4 unique types of molecules in this entry. The entry contains 19112 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

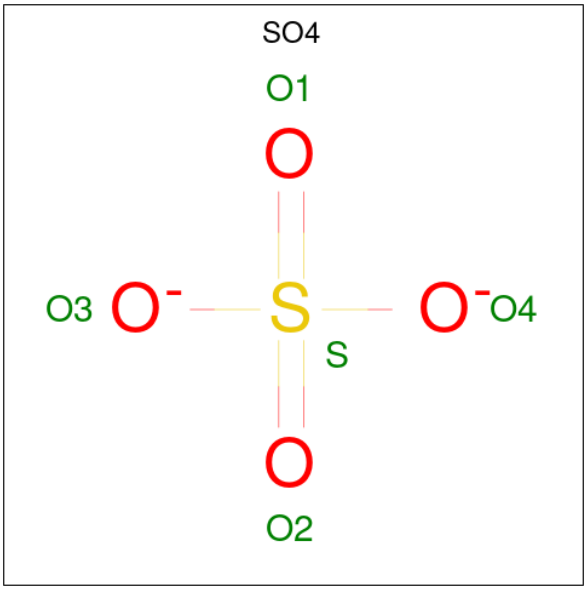
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	4	0
			3040	1930	531	566	13			
1	B	394	Total	C	N	O	S	0	4	0
			3036	1928	529	566	13			
1	C	394	Total	C	N	O	S	0	3	0
			3028	1922	524	569	13			
1	D	338	Total	C	N	O	S	0	2	0
			2571	1624	446	487	14			
1	E	393	Total	C	N	O	S	0	3	0
			3018	1917	526	564	11			
1	F	393	Total	C	N	O	S	0	4	0
			3029	1925	529	564	11			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: 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	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	F	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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			

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

- Molecule 4 is water.

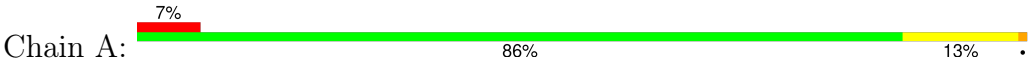
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	461	Total O 461 461	0	3
4	B	296	Total O 296 296	0	1
4	C	276	Total O 276 276	0	0
4	D	73	Total O 73 73	0	0
4	E	2	Total O 2 2	0	0
4	F	1	Total O 1 1	0	0

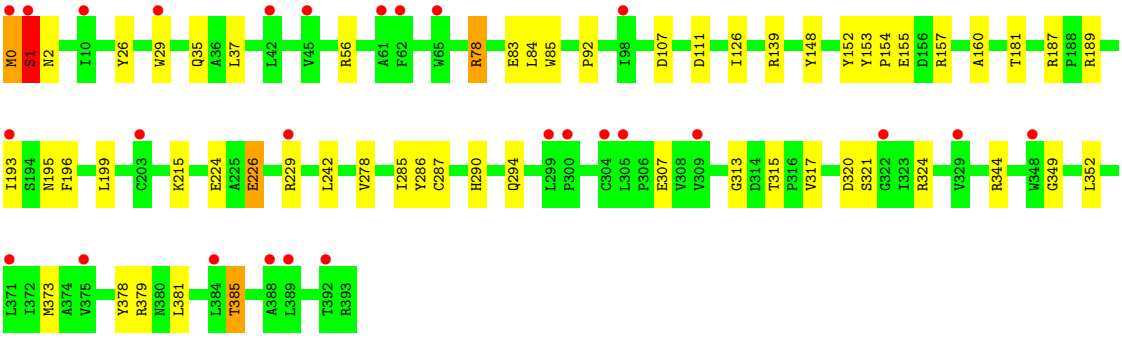
3 Residue-property plots (i)

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

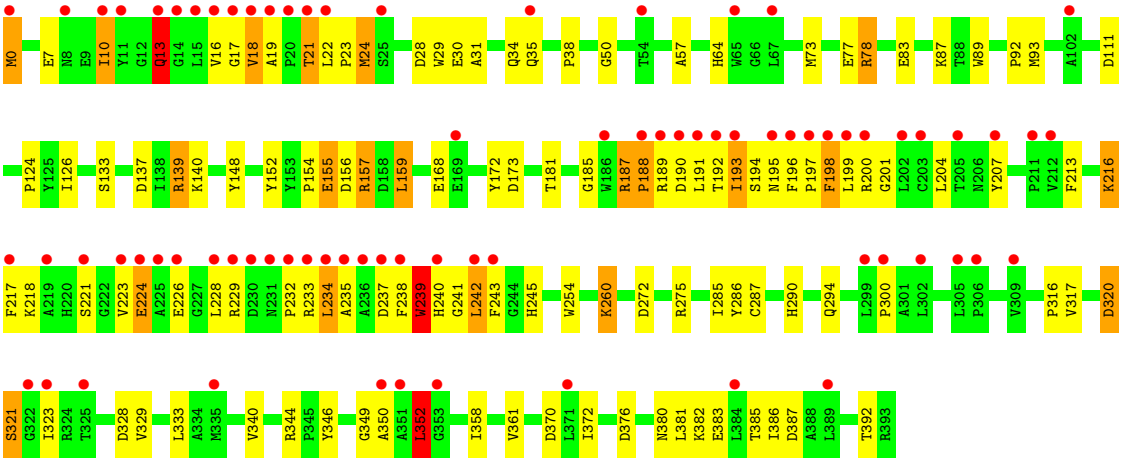
Chain A:





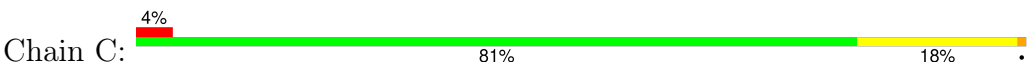
• Molecule 1: Lactate 2-monooxygenase

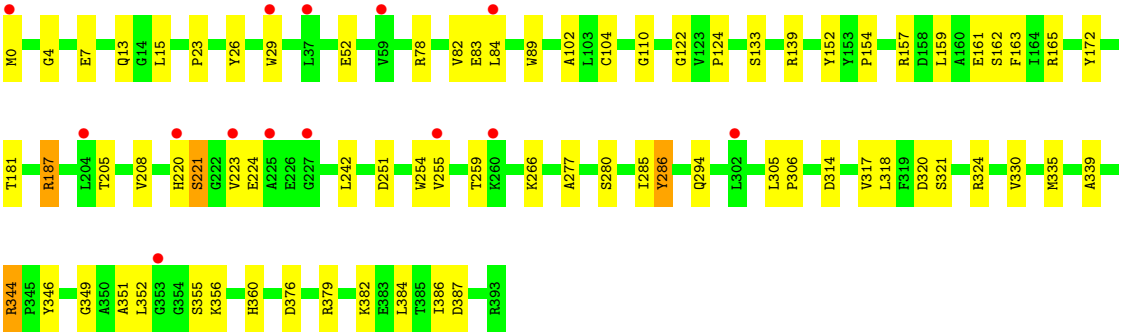
Chain B:



• Molecule 1: Lactate 2-monooxygenase

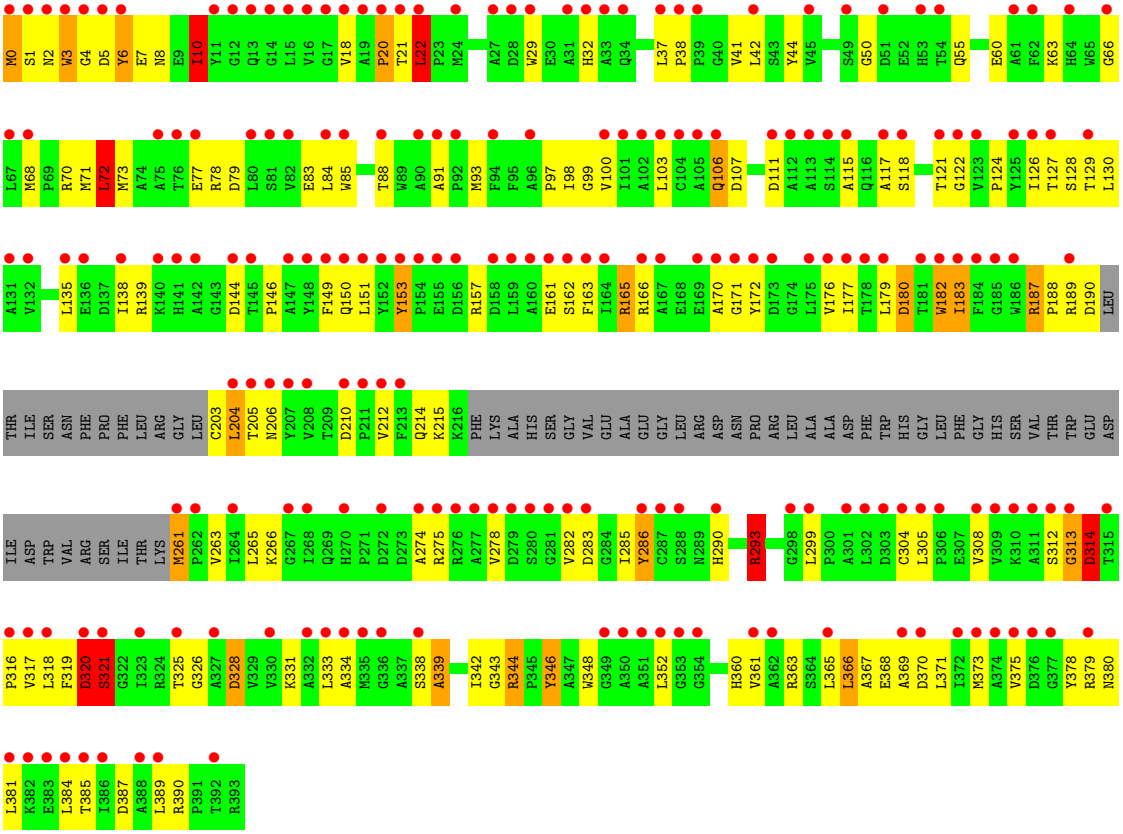
Chain C:





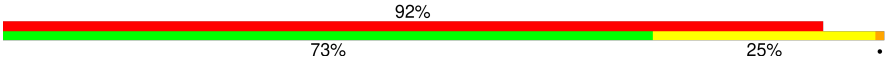
• Molecule 1: Lactate 2-monooxygenase

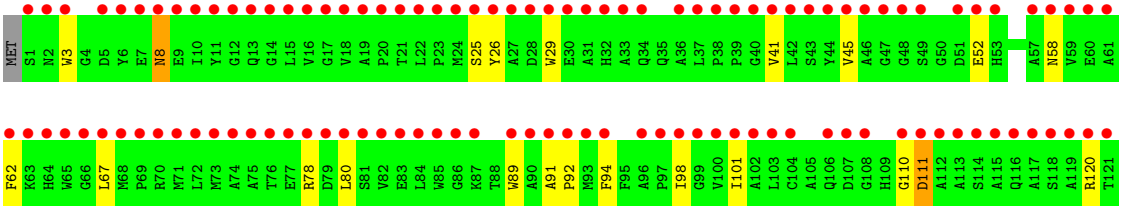
Chain D:

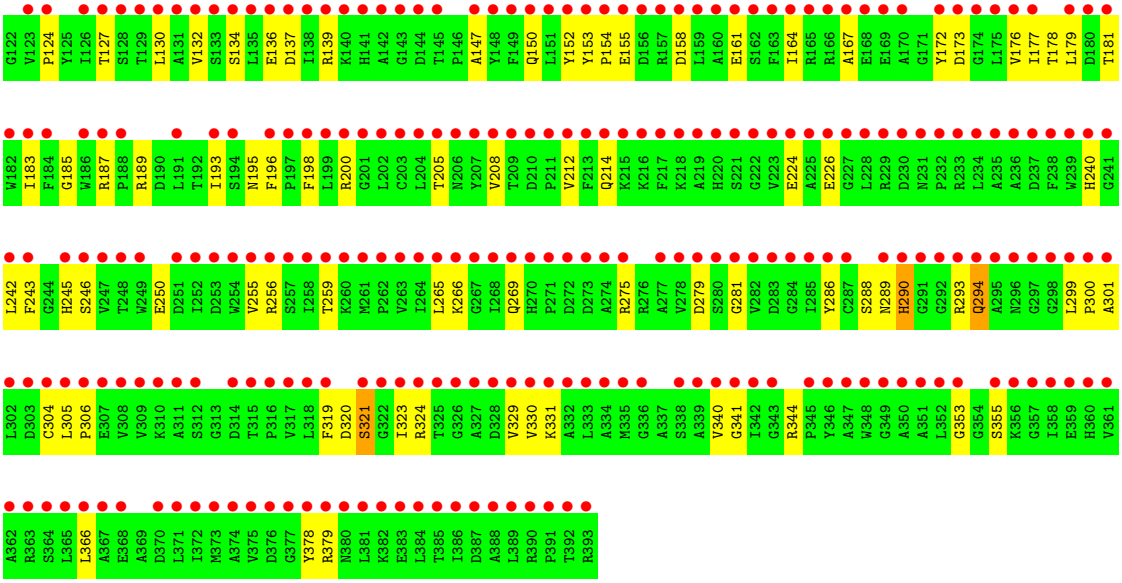


• Molecule 1: Lactate 2-monooxygenase

Chain E:

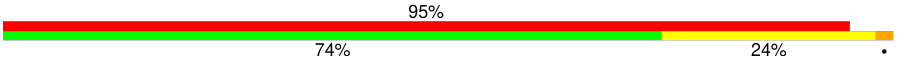


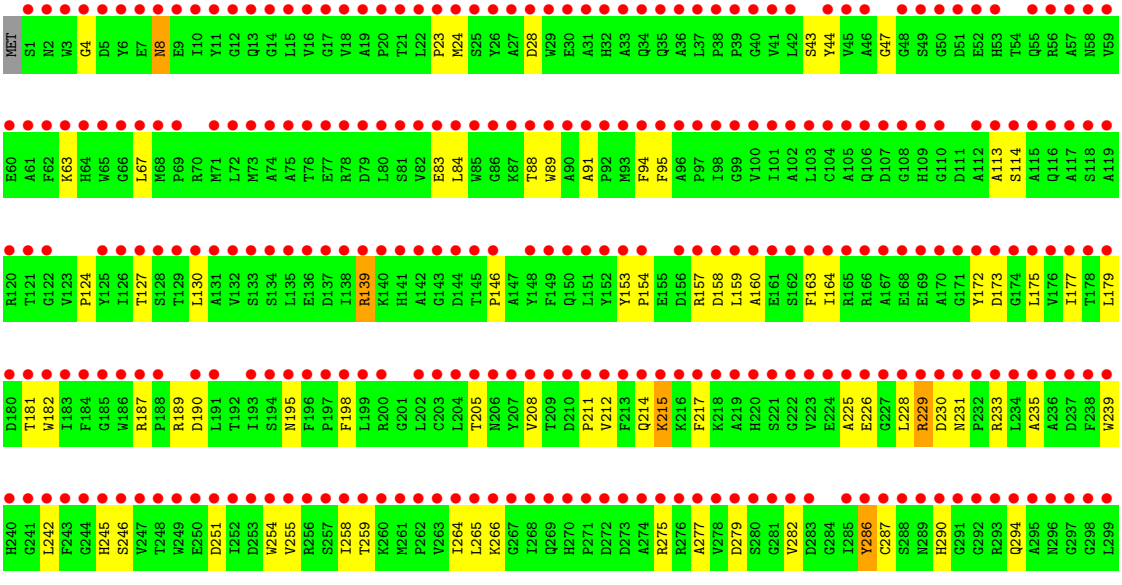




• Molecule 1: Lactate 2-monooxygenase

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	148.40Å 148.40Å 272.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.49 – 2.30 77.49 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.0 (77.49-2.30) 91.1 (77.49-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.218 , 0.272 0.225 , 0.276	Depositor DCC
R_{free} test set	12358 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 62.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	19112	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.93	2/3130 (0.1%)	0.91	4/4262 (0.1%)
1	B	0.84	1/3124 (0.0%)	0.95	9/4252 (0.2%)
1	C	0.80	0/3115	0.84	5/4244 (0.1%)
1	D	0.62	0/2638	0.80	7/3586 (0.2%)
1	E	0.35	0/3106	0.51	0/4229
1	F	0.35	0/3120	0.52	0/4248
All	All	0.69	3/18233 (0.0%)	0.78	25/24821 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	287	CYS	CB-SG	-6.79	1.70	1.82
1	B	287	CYS	CB-SG	-5.49	1.72	1.81
1	A	85	TRP	CB-CG	-5.33	1.40	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	352	LEU	CA-CB-CG	8.34	134.49	115.30
1	D	153	TYR	CA-CB-CG	7.97	128.54	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	204	LEU	CA-CB-CG	6.90	131.17	115.30
1	A	107	ASP	CB-CG-OD1	6.51	124.16	118.30
1	D	344	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	B	320	ASP	CB-CG-OD1	6.46	124.12	118.30
1	A	84	LEU	CA-CB-CG	-6.28	100.86	115.30
1	C	320	ASP	CB-CG-OD1	5.97	123.67	118.30
1	D	107	ASP	CB-CG-OD1	5.97	123.67	118.30
1	B	242	LEU	CB-CG-CD1	-5.96	100.87	111.00
1	B	187	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	C	376	ASP	CB-CG-OD1	5.83	123.54	118.30
1	B	187	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	C	15	LEU	CB-CG-CD1	-5.80	101.14	111.00
1	C	187	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	D	153	TYR	CB-CG-CD1	5.55	124.33	121.00
1	D	293	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	B	242	LEU	CB-CG-CD2	5.54	120.41	111.00
1	D	320	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	37	LEU	CB-CG-CD1	-5.41	101.81	111.00
1	B	328	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	B	320	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	C	346	TYR	CA-CB-CG	5.21	123.31	113.40
1	A	385	THR	CA-CB-CG2	-5.18	105.14	112.40
1	B	78	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3040	0	2944	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3036	0	2949	139	0
1	C	3028	0	2912	45	0
1	D	2571	0	2501	135	0
1	E	3018	0	2935	71	0
1	F	3029	0	2954	77	0
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	C	31	0	19	2	0
2	D	31	0	18	5	0
2	E	31	0	19	1	0
2	F	31	0	19	1	0
3	A	20	0	0	0	0
3	B	25	0	0	1	0
3	C	20	0	0	2	0
3	D	10	0	0	0	0
3	E	10	0	0	1	0
3	F	10	0	0	1	0
4	A	461	0	0	14	3
4	B	296	0	0	14	7
4	C	276	0	0	8	2
4	D	73	0	0	14	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
All	All	19112	0	17308	501	11

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 14.

All (501) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LEU:HD22	1:B:352:LEU:HD23	1.27	1.13
3:C:405:SO4:O2	4:C:1401:HOH:O	1.68	1.08
1:B:23:PRO:HB3	1:B:28:ASP:HB3	1.44	1.00
3:B:406:SO4:O4	4:B:501[A]:HOH:O	1.80	0.98
1:C:13:GLN:OE1	4:C:1402:HOH:O	1.81	0.96
1:F:63:LYS:NZ	3:F:403:SO4:O4	2.01	0.94
1:D:3:TRP:CZ3	1:D:91:ALA:HB2	2.04	0.92
1:C:314:ASP:OD1	4:C:1403:HOH:O	1.89	0.90
1:A:215:LYS:NZ	4:A:501:HOH:O	2.06	0.86
1:E:183:ILE:O	1:E:294:GLN:NE2	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:ASP:OD2	4:D:501:HOH:O	1.95	0.84
1:F:226:GLU:O	1:F:230:ASP:N	2.12	0.82
1:D:328:ASP:OD2	4:D:502:HOH:O	1.98	0.80
1:B:23:PRO:HB3	1:B:28:ASP:CB	2.12	0.80
1:C:187:ARG:NH2	1:C:294:GLN:OE1	2.14	0.79
1:E:275:ARG:NH1	1:E:279:ASP:OD2	2.15	0.79
1:F:225:ALA:O	1:F:229:ARG:N	2.16	0.78
1:B:188:PRO:HA	1:B:191:LEU:HD12	1.65	0.78
1:B:349:GLY:HA2	1:B:352:LEU:HD13	1.63	0.78
1:B:238:PHE:O	1:B:240:HIS:N	2.17	0.77
1:B:191:LEU:O	1:B:194:SER:OG	2.01	0.76
1:B:233:ARG:O	1:B:235:ALA:N	2.20	0.75
1:B:38:PRO:HG3	1:D:20:PRO:HD2	1.69	0.74
1:B:187:ARG:O	1:B:191:LEU:HG	1.88	0.74
1:A:385:THR:OG1	4:A:502:HOH:O	2.07	0.73
1:F:114:SER:OG	1:F:358:ILE:HD13	1.89	0.73
1:A:226:GLU:OE2	1:A:229:ARG:NH2	2.21	0.73
1:C:221:SER:OG	1:C:223:VAL:HG13	1.89	0.73
1:D:320:ASP:OD2	2:D:401:FMN:O3'	2.03	0.72
1:D:3:TRP:CH2	1:D:91:ALA:HB2	2.24	0.72
1:F:319:PHE:HE2	1:F:323:ILE:HD11	1.55	0.71
1:B:385:THR:OG1	1:B:387:ASP:OD1	2.08	0.71
1:B:10:ILE:O	1:B:10:ILE:HG13	1.91	0.71
1:D:21:THR:HG22	1:D:21:THR:O	1.90	0.70
1:B:173:ASP:OD1	4:B:503:HOH:O	2.10	0.70
1:B:155:GLU:CB	1:B:242:LEU:HD11	2.22	0.70
1:B:10:ILE:HG21	1:B:24:MET:CE	2.22	0.70
1:E:250:GLU:N	1:E:250:GLU:OE1	2.25	0.70
1:D:313:GLY:O	1:F:275:ARG:NH1	2.25	0.69
1:F:319:PHE:CE2	1:F:323:ILE:HD11	2.27	0.69
1:A:29[B]:TRP:CE3	1:A:352:LEU:HD12	2.28	0.69
1:C:154:PRO:HG3	1:C:159:LEU:HD12	1.73	0.69
1:D:4:GLY:N	1:D:370:ASP:OD2	2.26	0.69
1:B:168:GLU:OE1	4:B:502:HOH:O	2.10	0.68
1:B:10:ILE:HD13	1:B:24:MET:HE3	1.74	0.68
1:F:208:VAL:O	1:F:214:GLN:NE2	2.26	0.68
1:B:216:LYS:HE2	1:B:216:LYS:HA	1.76	0.68
1:F:212:VAL:O	1:F:215:LYS:N	2.27	0.67
1:A:187[A]:ARG:NH1	4:A:510[A]:HOH:O	2.24	0.67
1:F:255:VAL:O	1:F:259:THR:HG22	1.94	0.67
1:B:193:ILE:HD11	1:B:195:ASN:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:HIS:O	1:D:293:ARG:HB2	1.94	0.67
1:E:164:ILE:HD13	1:E:255:VAL:HG13	1.78	0.66
1:B:18:VAL:HG13	1:D:38:PRO:HG2	1.77	0.66
1:B:386:ILE:HD11	4:B:790:HOH:O	1.96	0.66
1:D:263:VAL:N	1:D:283:ASP:OD2	2.27	0.66
1:B:155:GLU:CB	1:B:242:LEU:CD1	2.74	0.66
1:D:320:ASP:O	1:D:321:SER:HB2	1.96	0.65
1:B:155:GLU:N	1:B:242:LEU:HD11	2.12	0.65
1:A:155:GLU:OE1	4:A:503:HOH:O	2.13	0.65
1:B:22:LEU:HD22	1:B:352:LEU:CD2	2.16	0.65
1:B:239:TRP:HA	1:B:239:TRP:CE3	2.31	0.65
1:B:155:GLU:HB3	1:B:242:LEU:CD1	2.28	0.64
1:B:155:GLU:HB3	1:B:242:LEU:HD11	1.80	0.64
1:E:136:GLU:OE1	1:E:136:GLU:N	2.30	0.63
1:F:84:LEU:HD12	1:F:89:TRP:CE2	2.33	0.63
1:B:18:VAL:HG13	1:D:38:PRO:CD	2.28	0.63
1:D:21:THR:O	1:D:22:LEU:HB2	1.98	0.63
1:B:155:GLU:H	1:B:242:LEU:CD1	2.12	0.63
1:E:255:VAL:O	1:E:259:THR:HG22	1.98	0.63
1:D:304:CYS:O	1:D:308:VAL:HG23	1.99	0.62
1:F:225:ALA:HA	1:F:228:LEU:HB3	1.81	0.62
1:B:193:ILE:HD11	1:B:195:ASN:CB	2.29	0.62
1:B:73:MET:HE3	4:B:557:HOH:O	1.98	0.62
1:D:42:LEU:HD22	4:D:510:HOH:O	1.99	0.62
1:D:6:TYR:O	1:D:10:ILE:HD11	2.00	0.62
1:C:266:LYS:HD2	1:C:286:TYR:CE2	2.36	0.61
1:F:287:CYS:N	1:F:318:LEU:O	2.31	0.61
1:D:3:TRP:HZ3	1:D:91:ALA:HB2	1.65	0.61
1:A:29[B]:TRP:CZ3	1:A:352:LEU:HD12	2.36	0.61
1:B:18:VAL:HG12	1:B:19:ALA:N	2.16	0.61
1:F:83:GLU:OE1	1:F:88:THR:OG1	2.17	0.60
1:D:117:ALA:O	1:D:121:THR:HG23	2.02	0.60
1:B:155:GLU:CA	1:B:242:LEU:HD11	2.31	0.60
1:B:157:ARG:HG2	1:B:254:TRP:CH2	2.36	0.60
1:B:223:VAL:HG11	1:B:234:LEU:HD11	1.82	0.60
1:D:139:ARG:NH2	1:D:171:GLY:O	2.35	0.60
1:E:134:SER:OG	1:E:137:ASP:OD2	2.18	0.60
1:B:189:ARG:O	1:B:193:ILE:HG23	2.02	0.60
1:B:139[B]:ARG:HG2	1:B:172:TYR:CE1	2.37	0.60
1:F:177:ILE:HD11	1:F:255:VAL:HG11	1.83	0.60
1:B:18:VAL:HG13	1:D:38:PRO:CG	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:GLY:O	1:D:189:ARG:NH1	2.35	0.59
1:E:52:GLU:OE2	1:E:189:ARG:NH2	2.31	0.59
1:B:10:ILE:HG21	1:B:24:MET:HE1	1.82	0.59
1:D:135:LEU:N	1:D:206:ASN:OD1	2.33	0.59
1:B:10:ILE:HD13	1:B:24:MET:CE	2.32	0.59
1:B:21:THR:HG21	4:B:744:HOH:O	2.01	0.59
1:B:157:ARG:HG2	1:B:254:TRP:CZ2	2.37	0.59
1:D:97:PRO:O	2:D:401:FMN:O2'	2.14	0.59
1:B:181:THR:HG21	1:B:290:HIS:CE1	2.38	0.58
1:B:139[B]:ARG:HG2	1:B:172:TYR:CZ	2.38	0.58
1:D:139:ARG:NE	1:D:171:GLY:O	2.35	0.58
1:E:299:LEU:HD21	1:E:304:CYS:SG	2.43	0.58
1:D:352:LEU:N	1:D:352:LEU:HD12	2.18	0.58
1:C:139:ARG:HG2	1:C:172:TYR:CZ	2.38	0.58
1:B:187:ARG:NH2	1:B:294:GLN:OE1	2.36	0.58
1:D:32:HIS:HB2	1:D:352:LEU:HD21	1.86	0.58
1:F:318:LEU:HD22	1:F:339:ALA:HB3	1.85	0.57
1:D:127:THR:HG22	1:D:138:ILE:HG21	1.86	0.57
1:B:200:ARG:NH2	4:B:509:HOH:O	2.31	0.57
1:C:251:ASP:OD1	4:C:1404:HOH:O	2.17	0.57
1:D:385:THR:HG21	4:D:541:HOH:O	2.04	0.57
1:F:23:PRO:HB3	1:F:28:ASP:HB3	1.87	0.57
1:F:114:SER:HG	1:F:346:TYR:HE2	1.52	0.57
1:F:317:VAL:O	1:F:338:SER:N	2.37	0.56
1:B:22:LEU:HB3	1:B:23:PRO:CD	2.34	0.56
1:C:266:LYS:HA	1:C:286:TYR:HB3	1.86	0.56
1:A:2:ASN:OD1	4:A:504:HOH:O	2.18	0.56
1:D:126:ILE:HD11	4:D:562:HOH:O	2.05	0.56
1:B:10:ILE:CD1	1:B:24:MET:CE	2.83	0.56
1:B:87:LYS:HE3	4:B:503:HOH:O	2.06	0.56
1:D:334:ALA:HB2	1:D:384:LEU:HG	1.88	0.56
1:E:155:GLU:N	1:E:242:LEU:O	2.34	0.56
1:D:348:TRP:O	1:D:352:LEU:CD1	2.54	0.56
1:B:196:PHE:CE1	1:B:198:PHE:CD2	2.94	0.55
1:D:139:ARG:CZ	1:D:171:GLY:O	2.55	0.55
1:B:10:ILE:CD1	1:B:24:MET:HE3	2.37	0.55
1:D:293:ARG:CZ	2:D:401:FMN:HM82	2.37	0.55
1:B:201:GLY:O	1:B:232:PRO:HB2	2.06	0.55
1:D:326:GLY:HA3	1:D:368:GLU:HB3	1.88	0.55
1:B:152:TYR:HE1	1:B:181:THR:HG1	1.53	0.55
1:B:350:ALA:HB2	1:B:358:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:GLN:CD	1:D:106:GLN:H	2.10	0.55
1:D:266:LYS:HA	1:D:286:TYR:HB3	1.89	0.55
1:D:328:ASP:N	1:D:328:ASP:OD1	2.39	0.54
1:A:285:ILE:O	1:A:317:VAL:HA	2.08	0.54
1:C:159:LEU:HD13	1:C:159:LEU:O	2.08	0.54
1:B:155:GLU:OE1	1:B:245:HIS:ND1	2.30	0.54
1:B:387:ASP:OD1	1:B:387:ASP:N	2.41	0.54
1:B:216:LYS:HD3	1:B:216:LYS:O	2.07	0.54
1:B:241:GLY:O	1:B:243:PHE:N	2.40	0.54
1:C:161:GLU:OE2	1:C:165:ARG:NH2	2.41	0.53
1:E:67:LEU:HD11	1:E:378:TYR:CE2	2.43	0.53
1:F:215:LYS:HG3	1:F:215:LYS:O	2.07	0.53
1:A:56:ARG:HD3	4:A:849:HOH:O	2.08	0.53
1:B:10:ILE:HD12	1:B:24:MET:HE2	1.91	0.53
1:B:190:ASP:O	1:B:194:SER:HA	2.08	0.53
1:D:0:MET:O	1:D:2:ASN:N	2.39	0.53
1:B:64:HIS:HA	1:B:392:THR:OG1	2.09	0.53
1:D:111:ASP:OD1	1:D:111:ASP:N	2.36	0.53
1:E:130:LEU:HD13	1:E:198:PHE:CE1	2.44	0.53
1:F:164:ILE:HD13	1:F:255:VAL:HG13	1.91	0.53
1:C:29[B]:TRP:CZ3	1:C:349:GLY:HA2	2.44	0.53
1:E:196:PHE:O	1:E:200:ARG:NH1	2.41	0.53
1:B:156:ASP:H	1:B:242:LEU:HD21	1.74	0.53
1:F:44:TYR:O	1:F:187[B]:ARG:NH2	2.41	0.53
1:A:92:PRO:HG3	1:A:381:LEU:HD11	1.91	0.53
1:F:181[B]:THR:HG22	1:F:294:GLN:HG3	1.91	0.53
1:B:240:HIS:O	1:B:243:PHE:N	2.42	0.53
1:D:3:TRP:CZ3	1:D:91:ALA:CB	2.88	0.53
1:D:93:MET:CE	1:D:366:LEU:HD13	2.39	0.53
1:D:274:ALA:HB2	1:D:308:VAL:HG13	1.90	0.53
1:F:212:VAL:HA	1:F:215:LYS:HB3	1.91	0.52
1:B:285:ILE:O	1:B:317:VAL:HA	2.10	0.52
1:D:66:GLY:O	1:D:390:ARG:N	2.42	0.52
1:D:122:GLY:O	1:D:124:PRO:HD3	2.09	0.52
1:E:58:ASN:OD1	1:E:300:PRO:HA	2.09	0.52
1:D:348:TRP:O	1:D:352:LEU:HD12	2.10	0.52
1:E:150:GLN:HA	1:E:176:VAL:HB	1.91	0.52
1:D:162:SER:OG	1:D:210:ASP:OD2	2.12	0.52
1:B:238:PHE:O	1:B:239:TRP:C	2.47	0.52
1:B:243:PHE:CD1	1:B:243:PHE:O	2.64	0.52
1:D:50:GLY:O	1:D:189:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:LEU:HD21	4:D:562:HOH:O	2.10	0.51
1:B:320:ASP:O	1:B:321:SER:HB2	2.10	0.51
1:D:128:SER:HA	1:D:150:GLN:OE1	2.10	0.51
1:D:32:HIS:CB	1:D:352:LEU:HD21	2.40	0.51
1:D:187:ARG:NH2	1:D:293:ARG:HG2	2.25	0.51
1:E:111:ASP:OD2	1:E:132:VAL:N	2.39	0.51
1:A:29[B]:TRP:HZ3	1:A:352:LEU:HB2	1.75	0.51
1:D:115:ALA:HA	1:D:118:SER:HB3	1.93	0.51
1:E:256:ARG:NH2	1:E:281:GLY:O	2.43	0.51
1:A:181:THR:O	1:A:181:THR:HG22	2.09	0.51
1:D:32:HIS:HB3	1:D:352:LEU:HG	1.92	0.51
1:D:177:ILE:HD12	1:D:263:VAL:HG13	1.92	0.51
1:E:185:GLY:N	1:E:294:GLN:OE1	2.27	0.51
1:F:228:LEU:HD13	1:F:235:ALA:HB2	1.92	0.51
1:D:55:GLN:OE1	1:D:344:ARG:NH2	2.43	0.51
1:E:205:THR:HA	1:E:208[A]:VAL:HG22	1.93	0.51
1:F:217:PHE:CE2	1:F:235:ALA:HB2	2.45	0.51
1:B:237:ASP:O	1:B:238:PHE:C	2.50	0.50
1:E:130:LEU:HD13	1:E:198:PHE:CZ	2.47	0.50
1:F:245:HIS:NE2	1:F:251:ASP:OD2	2.44	0.50
1:A:307:GLU:OE1	4:A:505:HOH:O	2.20	0.50
1:B:193:ILE:CD1	1:B:195:ASN:HB2	2.40	0.50
1:D:344:ARG:HD3	2:D:401:FMN:O2P	2.12	0.50
1:E:8:ASN:OD1	1:E:8:ASN:N	2.44	0.50
1:F:89:TRP:HB3	1:F:91:ALA:O	2.11	0.50
1:F:179:LEU:HD11	1:F:265:LEU:HB3	1.92	0.50
1:B:185:GLY:HA3	1:B:294:GLN:O	2.11	0.50
1:B:223:VAL:O	1:B:224:GLU:CG	2.59	0.50
2:C:401:FMN:H9	2:C:401:FMN:O4'	2.12	0.50
1:E:80:LEU:HB3	1:E:92:PRO:HD3	1.93	0.50
1:B:196:PHE:CE1	1:B:198:PHE:HD2	2.28	0.50
1:D:44:TYR:CD1	1:D:190:ASP:HB3	2.47	0.50
1:D:139:ARG:HB2	1:D:172:TYR:CZ	2.46	0.50
1:E:179:LEU:HD11	1:E:265:LEU:HB3	1.93	0.50
1:E:305:LEU:HB3	1:E:306:PRO:HD3	1.93	0.50
1:F:181[B]:THR:HG21	1:F:290:HIS:CE1	2.47	0.50
1:B:38:PRO:HG3	1:D:20:PRO:CD	2.41	0.50
1:F:67:LEU:HD11	1:F:378:TYR:CE2	2.47	0.50
1:B:137:ASP:OD2	4:B:504:HOH:O	2.19	0.50
1:B:18:VAL:HG12	1:B:19:ALA:H	1.77	0.49
1:D:93:MET:HE1	1:D:366:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:THR:CG2	1:B:290:HIS:CE1	2.94	0.49
1:C:122:GLY:O	1:C:124:PRO:HD3	2.12	0.49
1:E:167:ALA:O	1:E:172:TYR:HB2	2.12	0.49
1:B:323[B]:ILE:HG13	1:B:340[B]:VAL:CG1	2.42	0.49
1:C:344:ARG:HD3	2:C:401:FMN:C8M	2.43	0.49
1:E:3:TRP:HD1	1:E:80:LEU:HD22	1.76	0.49
1:E:329:VAL:HG13	1:E:340[A]:VAL:HG21	1.94	0.49
1:B:188:PRO:CA	1:B:191:LEU:HD12	2.38	0.49
1:D:334:ALA:HB3	1:D:389:LEU:HD11	1.95	0.49
1:D:285:ILE:O	1:D:317:VAL:HA	2.13	0.49
1:F:266:LYS:HA	1:F:286:TYR:HB3	1.94	0.49
1:A:126:ILE:HG12	1:A:148:TYR:HB2	1.95	0.49
1:E:290:HIS:NE2	3:E:403:SO4:O2	2.44	0.49
1:E:193:ILE:CD1	1:E:195:ASN:HB2	2.43	0.49
1:C:159:LEU:HD11	1:C:163:PHE:CE2	2.48	0.49
1:F:228:LEU:HD13	1:F:235:ALA:CB	2.43	0.49
1:C:29[B]:TRP:CE3	1:C:352:LEU:HD12	2.48	0.49
1:D:79:ASP:HB3	1:D:380:ASN:HB3	1.95	0.49
1:A:1[A]:SER:O	4:A:504:HOH:O	2.18	0.48
1:D:265:LEU:HD11	1:D:282:VAL:HG21	1.94	0.48
1:E:305:LEU:HD13	1:E:319:PHE:HD1	1.77	0.48
1:B:197:PRO:O	1:B:200:ARG:N	2.37	0.48
1:B:213:PHE:HE1	1:B:228:LEU:CD2	2.25	0.48
1:C:187:ARG:NH2	3:C:402:SO4:O2	2.32	0.48
1:F:319:PHE:CD2	1:F:332:ALA:HB1	2.48	0.48
1:B:380:ASN:OD1	1:B:383:GLU:HG3	2.13	0.48
1:E:158:ASP:O	1:E:212:VAL:HG21	2.13	0.48
1:C:305:LEU:HB3	1:C:306:PRO:HD3	1.95	0.48
1:D:29:TRP:CD2	1:D:361:VAL:HG22	2.48	0.48
1:E:288:SER:OG	1:E:320:ASP:OD1	2.21	0.48
1:F:158:ASP:O	1:F:212:VAL:HG21	2.13	0.48
1:F:229:ARG:NH1	1:F:230:ASP:OD1	2.46	0.48
1:B:187:ARG:O	1:B:191:LEU:CG	2.59	0.48
1:E:98:ILE:HG22	1:E:101:ILE:N	2.29	0.48
1:A:193:ILE:HG13	1:A:195:ASN:HB2	1.94	0.48
1:D:278:VAL:HG21	1:D:312:SER:HA	1.95	0.48
1:D:338:SER:O	1:D:339:ALA:HB2	2.14	0.48
1:D:379:ARG:HB3	4:D:530:HOH:O	2.12	0.48
1:B:0:MET:O	1:B:0:MET:SD	2.72	0.48
1:D:161:GLU:O	1:D:165:ARG:HB2	2.14	0.48
1:D:320:ASP:OD1	1:D:320:ASP:C	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:320:ASP:OD1	1:E:320:ASP:C	2.52	0.48
1:B:22:LEU:HB3	1:B:23:PRO:HD2	1.96	0.47
1:B:228:LEU:HD12	1:B:232:PRO:HA	1.95	0.47
1:D:182:TRP:CE3	1:D:183:ILE:HB	2.49	0.47
1:E:98:ILE:HG23	2:E:401:FMN:C6	2.43	0.47
1:E:181:THR:HG21	1:E:290:HIS:CE1	2.49	0.47
1:B:223:VAL:O	1:B:224:GLU:HG2	2.13	0.47
1:E:3:TRP:CD1	1:E:80:LEU:HD22	2.49	0.47
1:A:29[B]:TRP:CZ3	1:A:349:GLY:HA2	2.49	0.47
1:D:124:PRO:HB3	1:D:146:PRO:O	2.15	0.47
1:E:41:VAL:O	1:E:45:VAL:HG23	2.15	0.47
1:C:318:LEU:HD22	1:C:339:ALA:HB3	1.97	0.47
1:D:342:ILE:O	1:D:346:TYR:CE2	2.68	0.47
1:D:348:TRP:CE3	1:D:348:TRP:HA	2.49	0.47
1:F:277:ALA:HB1	1:F:282:VAL:HG21	1.96	0.47
1:B:233:ARG:O	1:B:234:LEU:C	2.53	0.47
1:B:240:HIS:O	1:B:241:GLY:C	2.52	0.47
1:D:348:TRP:HA	1:D:348:TRP:HE3	1.79	0.47
1:E:305:LEU:HD13	1:E:319:PHE:CD1	2.49	0.47
1:A:154:PRO:HD2	1:A:160:ALA:HB2	1.97	0.47
1:B:111:ASP:OD1	1:B:111:ASP:N	2.48	0.47
1:C:4:GLY:O	1:C:7:GLU:HG2	2.14	0.47
1:E:111:ASP:OD1	1:E:111:ASP:N	2.44	0.47
1:F:67:LEU:HD11	1:F:378:TYR:CZ	2.49	0.47
1:F:305:LEU:HB3	1:F:306:PRO:HD3	1.95	0.47
1:A:242:LEU:HD12	1:A:242:LEU:C	2.34	0.47
1:A:313:GLY:O	4:A:506:HOH:O	2.20	0.47
1:D:342:ILE:O	1:D:346:TYR:CD2	2.68	0.47
1:B:13:GLN:O	1:B:16:VAL:HG13	2.14	0.47
1:B:323[A]:ILE:CD1	1:B:340[A]:VAL:HB	2.45	0.47
1:C:355:SER:HB3	4:C:1626:HOH:O	2.15	0.47
1:A:278:VAL:HG22	1:A:315:THR:HG21	1.97	0.47
1:B:50:GLY:O	1:B:188:PRO:HG2	2.15	0.47
1:B:217:PHE:CE2	1:B:223:VAL:CG2	2.98	0.46
1:D:44:TYR:HD1	1:D:190:ASP:HB3	1.80	0.46
1:D:93:MET:SD	1:D:342:ILE:HD11	2.55	0.46
1:D:369:ALA:O	1:D:373:MET:HG3	2.15	0.46
1:F:215:LYS:O	1:F:215:LYS:CG	2.62	0.46
1:D:85:TRP:NE1	1:D:283:ASP:O	2.46	0.46
1:D:314:ASP:OD1	1:D:314:ASP:C	2.53	0.46
1:E:26:TYR:CZ	1:E:324:ARG:HD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:ARG:NH2	1:E:355:SER:OG	2.35	0.46
1:E:329:VAL:HG22	1:E:340[A]:VAL:HG21	1.97	0.46
1:F:159:LEU:CA	1:F:212:VAL:HG11	2.45	0.46
1:C:26:TYR:CZ	1:C:324:ARG:HD2	2.51	0.46
1:C:52:GLU:HA	4:C:1556:HOH:O	2.16	0.46
1:C:159:LEU:HD13	1:C:159:LEU:C	2.36	0.46
1:E:154:PRO:HA	1:E:243:PHE:O	2.15	0.46
1:D:261:MET:HA	1:D:261:MET:CE	2.45	0.46
1:F:323:ILE:HD12	1:F:340:VAL:HG11	1.98	0.46
1:C:83[A]:GLU:OE1	4:C:1405:HOH:O	2.20	0.46
1:D:187:ARG:N	1:D:188:PRO:HD3	2.31	0.46
1:A:35:GLN:HA	4:A:517:HOH:O	2.15	0.46
1:B:13:GLN:O	1:B:17:GLY:N	2.48	0.46
1:D:68:MET:O	1:D:378:TYR:OH	2.23	0.46
1:E:187:ARG:HH12	1:E:293:ARG:CZ	2.28	0.46
1:B:18:VAL:HG11	1:D:41:VAL:HG21	1.97	0.46
1:C:29[B]:TRP:HZ2	1:C:360:HIS:HD2	1.64	0.46
1:C:159:LEU:HD11	1:C:163:PHE:CZ	2.51	0.46
1:D:70:ARG:HG3	4:D:520:HOH:O	2.16	0.46
1:D:150:GLN:HA	1:D:176:VAL:HB	1.97	0.46
1:F:242:LEU:HD12	1:F:242:LEU:C	2.36	0.46
1:B:18:VAL:O	1:B:19:ALA:C	2.54	0.45
1:B:92:PRO:HG3	1:B:381:LEU:HD11	1.98	0.45
1:E:299:LEU:HD12	1:E:300:PRO:HD2	1.96	0.45
1:B:234:LEU:C	1:B:234:LEU:HD13	2.36	0.45
1:C:356:LYS:HD2	4:C:1567:HOH:O	2.16	0.45
1:E:94:PHE:O	1:E:341:GLY:HA2	2.17	0.45
1:D:63:LYS:NZ	4:D:504:HOH:O	2.28	0.45
1:F:190:ASP:HB3	1:F:195:ASN:O	2.17	0.45
1:C:84:LEU:HD12	1:C:89:TRP:CD2	2.52	0.45
1:D:6:TYR:CE1	1:D:363:ARG:HD2	2.51	0.45
1:B:204:LEU:HD22	1:B:207:TYR:CD2	2.52	0.45
1:E:52:GLU:OE2	1:E:189:ARG:NE	2.46	0.45
1:F:226:GLU:O	1:F:229:ARG:N	2.50	0.45
1:A:0:MET:O	1:A:2:ASN:N	2.50	0.45
1:D:163:PHE:HE1	1:D:166:ARG:HH12	1.65	0.45
1:D:180:ASP:OD1	1:D:180:ASP:C	2.55	0.45
1:F:94:PHE:O	1:F:341:GLY:HA2	2.17	0.45
1:B:260:LYS:HD2	4:B:619:HOH:O	2.16	0.45
1:C:285:ILE:O	1:C:317:VAL:HA	2.17	0.45
1:D:313:GLY:O	1:D:314:ASP:HB3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:198:PHE:HB2	1:F:239:TRP:CH2	2.52	0.45
1:B:29:TRP:CZ3	1:B:361:VAL:HG13	2.52	0.44
1:F:265:LEU:HD11	1:F:282:VAL:HG21	2.00	0.44
1:D:5:ASP:O	1:D:367:ALA:HB2	2.17	0.44
1:D:371:LEU:O	1:D:375:VAL:HG23	2.17	0.44
1:B:196:PHE:HE1	1:B:198:PHE:CE2	2.35	0.44
1:B:31:ALA:O	1:B:35:GLN:HG2	2.17	0.44
1:E:52:GLU:CD	1:E:189:ARG:HH21	2.18	0.44
1:F:8:ASN:N	1:F:8:ASN:OD1	2.49	0.44
1:F:146:PRO:HA	1:F:173:ASP:OD2	2.18	0.44
1:F:231:ASN:O	1:F:233:ARG:N	2.50	0.44
1:B:77:GLU:OE1	4:B:505:HOH:O	2.21	0.44
1:D:71:MET:O	1:D:72:LEU:C	2.55	0.44
1:D:275:ARG:HD3	1:F:313:GLY:HA3	1.99	0.44
1:E:320:ASP:O	1:E:321:SER:CB	2.65	0.44
1:D:21:THR:O	1:D:21:THR:CG2	2.60	0.44
1:D:129:THR:OG1	1:D:151:LEU:HA	2.17	0.44
1:E:91:ALA:HB1	1:E:366:LEU:HD21	2.00	0.44
1:B:193:ILE:HG22	4:B:652:HOH:O	2.17	0.44
1:C:0:MET:O	1:C:0:MET:SD	2.76	0.44
1:E:153:TYR:CD1	1:E:245:HIS:HD2	2.36	0.44
1:A:196:PHE:CD2	1:A:199:LEU:HG	2.52	0.44
1:D:99:GLY:CA	1:D:130:LEU:HB2	2.48	0.44
1:F:84:LEU:HD12	1:F:89:TRP:CD2	2.53	0.44
1:A:78:ARG:O	4:A:504:HOH:O	2.21	0.44
1:A:373:MET:HB3	1:A:378:TYR:O	2.18	0.44
1:B:139[B]:ARG:CG	1:B:172:TYR:CE1	3.01	0.44
1:B:239:TRP:CE3	1:B:239:TRP:CA	3.00	0.44
1:E:240:HIS:O	1:E:240:HIS:CG	2.70	0.44
1:C:205:THR:HA	1:C:208:VAL:HG22	2.00	0.43
1:E:178:THR:HA	1:E:266:LYS:HB3	1.99	0.43
1:B:190:ASP:O	1:B:194:SER:CA	2.66	0.43
1:A:26:TYR:CE2	1:A:324:ARG:HD2	2.53	0.43
1:A:181:THR:OG1	1:A:290:HIS:CE1	2.70	0.43
1:A:189:ARG:HD3	4:A:861:HOH:O	2.18	0.43
1:D:3:TRP:CZ2	1:D:366:LEU:HD23	2.53	0.43
1:D:182:TRP:CZ3	1:D:183:ILE:HB	2.52	0.43
1:D:343:GLY:O	1:D:344:ARG:C	2.57	0.43
1:F:43:SER:OG	1:F:189:ARG:O	2.36	0.43
1:B:156:ASP:HB3	1:B:159:LEU:HB2	1.99	0.43
1:B:385:THR:CB	1:B:387:ASP:OD1	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:ALA:HB1	1:E:366:LEU:CD2	2.47	0.43
1:F:113:ALA:HB1	1:F:355:SER:HB2	1.99	0.43
1:F:320:ASP:O	1:F:321:SER:HB2	2.18	0.43
1:B:16:VAL:HG22	1:B:16:VAL:O	2.18	0.43
1:B:89:TRP:CD2	1:B:124:PRO:HG2	2.54	0.43
1:B:241:GLY:C	1:B:243:PHE:H	2.21	0.43
1:C:104:CYS:O	1:C:351:ALA:HA	2.19	0.43
1:C:220:HIS:O	1:C:220:HIS:CG	2.71	0.43
1:C:335:MET:HA	1:C:386:ILE:HD12	1.99	0.43
1:D:77:GLU:OE2	4:D:503:HOH:O	2.21	0.43
1:E:67:LEU:HD22	1:E:330:VAL:HG11	2.01	0.43
1:F:159:LEU:N	1:F:212:VAL:HG11	2.33	0.43
1:A:152:TYR:HE1	1:A:181:THR:HB	1.83	0.43
1:D:3:TRP:HZ3	1:D:91:ALA:CA	2.32	0.43
1:D:83:GLU:HG2	1:D:88:THR:OG1	2.18	0.43
1:A:226:GLU:HA	1:A:229:ARG:HG2	2.00	0.43
1:B:34:GLN:HB2	4:B:573:HOH:O	2.19	0.43
1:B:193:ILE:CG1	1:B:195:ASN:HB2	2.49	0.43
1:D:98:ILE:HG23	2:D:401:FMN:HM73	2.01	0.43
1:D:139:ARG:HG2	1:D:170:ALA:O	2.18	0.43
1:D:210:ASP:OD1	1:D:212:VAL:N	2.51	0.43
1:D:305:LEU:HD22	1:D:319:PHE:CD1	2.53	0.43
1:F:24:MET:SD	1:F:360:HIS:NE2	2.91	0.43
1:F:254:TRP:CZ2	1:F:258:ILE:HD13	2.54	0.43
2:F:401:FMN:N1	2:F:401:FMN:O2'	2.48	0.43
1:A:199:LEU:HD22	4:A:731:HOH:O	2.19	0.43
1:E:269:GLN:OE1	1:E:301:ALA:HA	2.19	0.43
1:D:71:MET:O	1:D:73:MET:N	2.52	0.42
1:E:89:TRP:CD2	1:E:124:PRO:HG2	2.54	0.42
1:E:177:ILE:HD11	1:E:255:VAL:HG11	2.01	0.42
1:B:23:PRO:CB	1:B:28:ASP:CB	2.89	0.42
1:F:4:GLY:HA3	1:F:371:LEU:HD21	2.01	0.42
1:A:26:TYR:HA	1:A:29[A]:TRP:CE3	2.54	0.42
1:A:320:ASP:C	1:A:320:ASP:OD1	2.57	0.42
1:B:154:PRO:HG3	1:B:159:LEU:HD13	2.02	0.42
1:D:0:MET:HE2	1:D:3:TRP:HA	2.01	0.42
1:D:179:LEU:HD12	4:D:505:HOH:O	2.18	0.42
1:F:127:THR:HG21	1:F:172:TYR:OH	2.19	0.42
1:A:294:GLN:OE1	4:A:507[B]:HOH:O	2.22	0.42
1:B:181:THR:HG21	1:B:290:HIS:HE1	1.82	0.42
1:C:102:ALA:HA	1:C:110:GLY:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:VAL:O	1:C:259:THR:HG22	2.20	0.42
1:B:10:ILE:CD1	1:B:24:MET:HE2	2.48	0.42
1:B:329:VAL:O	1:B:333:LEU:HG	2.19	0.42
1:C:181:THR:OG1	1:C:294:GLN:HG3	2.19	0.42
1:D:135:LEU:HD22	1:D:149:PHE:CE1	2.55	0.42
1:F:175:LEU:O	1:F:264:ILE:N	2.48	0.42
1:A:26:TYR:CZ	1:A:324:ARG:HD2	2.54	0.42
1:A:187[A]:ARG:HH21	1:A:294:GLN:HG2	1.84	0.42
1:B:382:LYS:HG2	4:B:671:HOH:O	2.19	0.42
1:D:10:ILE:HD13	1:D:360:HIS:CE1	2.55	0.42
1:D:83:GLU:CG	1:D:88:THR:OG1	2.68	0.42
1:E:26:TYR:HA	1:E:29:TRP:HB2	2.01	0.42
1:B:78:ARG:HE	1:B:370:ASP:CG	2.23	0.42
1:E:62:PHE:O	1:E:331:LYS:NZ	2.42	0.42
1:B:18:VAL:CG1	1:B:19:ALA:N	2.82	0.42
1:C:157:ARG:HG3	1:C:254:TRP:CH2	2.54	0.42
1:E:289:ASN:O	1:E:290:HIS:CB	2.68	0.42
1:F:211:PRO:HA	1:F:214:GLN:HB2	2.01	0.42
1:C:277:ALA:O	1:C:280:SER:HB2	2.19	0.41
1:D:4:GLY:HA2	1:D:367:ALA:HA	2.01	0.41
1:D:99:GLY:HA2	1:D:130:LEU:HB2	2.02	0.41
1:E:127:THR:HG23	1:E:127:THR:O	2.20	0.41
1:E:320:ASP:O	1:E:321:SER:HB2	2.19	0.41
1:F:47:GLY:O	1:F:187[B]:ARG:NH1	2.52	0.41
1:B:154:PRO:HB2	1:B:242:LEU:HG	2.03	0.41
1:B:223:VAL:HG21	1:B:234:LEU:HG	2.01	0.41
1:E:155:GLU:HB2	1:E:242:LEU:HA	2.02	0.41
1:F:139:ARG:HG2	1:F:172:TYR:CE2	2.55	0.41
1:F:139:ARG:HG2	1:F:172:TYR:CZ	2.56	0.41
1:B:93:MET:O	1:B:124:PRO:HD2	2.20	0.41
1:D:127:THR:HG21	1:D:172:TYR:OH	2.20	0.41
1:D:265:LEU:CD1	1:D:282:VAL:HG21	2.49	0.41
1:F:160:ALA:O	1:F:163:PHE:N	2.54	0.41
1:F:205:THR:O	1:F:205:THR:HG22	2.19	0.41
1:F:332:ALA:HB3	1:F:340:VAL:HG21	2.01	0.41
1:B:223:VAL:O	1:B:224:GLU:OE1	2.38	0.41
1:B:320:ASP:O	1:B:321:SER:CB	2.67	0.41
1:E:379:ARG:CZ	1:E:379:ARG:HB2	2.49	0.41
1:B:188:PRO:O	1:B:192:THR:N	2.32	0.41
1:B:240:HIS:O	1:B:243:PHE:HB3	2.21	0.41
1:D:50:GLY:O	1:D:189:ARG:CZ	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:LEU:HD21	1:D:316:PRO:HB3	2.02	0.41
1:D:278:VAL:HG12	1:F:279:ASP:OD1	2.21	0.41
1:F:95:PHE:CZ	1:F:358:ILE:HG22	2.56	0.41
1:F:154:PRO:CB	1:F:242:LEU:O	2.68	0.41
1:B:30:GLU:O	1:B:31:ALA:C	2.58	0.41
1:C:161:GLU:O	1:C:165:ARG:HG3	2.21	0.41
1:D:100:VAL:HB	1:D:103:LEU:HD12	2.02	0.41
1:F:94:PHE:HE1	1:F:286:TYR:OH	2.04	0.41
1:C:23:PRO:HB2	1:C:29[A]:TRP:CD1	2.55	0.41
1:D:331:LYS:NZ	4:D:512:HOH:O	2.47	0.41
1:D:361:VAL:O	1:D:365:LEU:HG	2.21	0.41
1:B:57:ALA:HB1	1:B:300:PRO:HG3	2.02	0.41
1:D:2:ASN:O	1:D:2:ASN:CG	2.59	0.41
1:D:333:LEU:HD13	1:D:381:LEU:CD2	2.50	0.41
1:E:161:GLU:O	1:E:164:ILE:N	2.54	0.41
1:B:199:LEU:HD23	1:B:199:LEU:HA	1.85	0.41
1:C:78:ARG:HA	1:C:379:ARG:O	2.21	0.41
1:D:6:TYR:HE2	1:D:360:HIS:HD1	1.67	0.41
1:D:70:ARG:CG	4:D:520:HOH:O	2.68	0.41
1:E:323:ILE:HD12	1:E:340[B]:VAL:HG11	2.03	0.41
1:F:130[B]:LEU:HD13	1:F:198:PHE:CZ	2.55	0.41
1:D:7:GLU:OE2	1:D:371:LEU:CD1	2.69	0.41
1:E:147:ALA:N	1:E:173:ASP:OD2	2.48	0.41
1:F:124:PRO:HB3	1:F:146:PRO:O	2.20	0.41
1:B:188:PRO:O	1:B:191:LEU:N	2.53	0.40
1:B:272[B]:ASP:OD1	1:B:275:ARG:NE	2.43	0.40
1:B:372:ILE:O	1:B:376:ASP:HB2	2.21	0.40
1:C:82:VAL:HG13	1:C:89:TRP:HB2	2.02	0.40
1:A:111:ASP:OD1	1:A:111:ASP:N	2.53	0.40
1:B:126:ILE:HG12	1:B:148:TYR:HB2	2.03	0.40
1:C:330:VAL:HG13	1:C:384:LEU:HD21	2.02	0.40
1:D:29:TRP:CE3	1:D:361:VAL:HG22	2.56	0.40
1:D:37:LEU:HB2	4:D:510:HOH:O	2.21	0.40
1:B:372:ILE:HD13	1:B:372:ILE:HG21	1.89	0.40
1:F:182:TRP:CE2	1:F:246:SER:OG	2.61	0.40
1:B:152:TYR:O	1:B:154:PRO:HD3	2.21	0.40
1:D:183:ILE:HG23	1:D:183:ILE:O	2.22	0.40

All (11) 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:B:786:HOH:O	4:B:791:HOH:O[4_455]	1.94	0.26
4:B:734:HOH:O	4:B:787:HOH:O[3_555]	1.95	0.25
4:A:750:HOH:O	4:A:819:HOH:O[3_545]	2.04	0.16
4:A:554:HOH:O	4:A:633:HOH:O[3_545]	2.07	0.13
4:C:1415:HOH:O	4:C:1453:HOH:O[3_545]	2.07	0.13
4:B:578:HOH:O	4:B:729:HOH:O[3_555]	2.08	0.12
4:B:688:HOH:O	4:B:732:HOH:O[3_555]	2.09	0.11
4:B:718:HOH:O	4:B:769:HOH:O[4_455]	2.09	0.11
4:C:1446:HOH:O	4:C:1578:HOH:O[4_555]	2.09	0.11
4:A:774:HOH:O	4:B:661:HOH:O[7_555]	2.15	0.05
4:B:727:HOH:O	4:B:751:HOH:O[4_455]	2.16	0.04

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	396/394 (100%)	385 (97%)	8 (2%)	3 (1%)	19 23
1	B	396/394 (100%)	360 (91%)	27 (7%)	9 (2%)	6 5
1	C	395/394 (100%)	385 (98%)	8 (2%)	2 (0%)	29 35
1	D	334/394 (85%)	295 (88%)	28 (8%)	11 (3%)	4 2
1	E	394/394 (100%)	365 (93%)	24 (6%)	5 (1%)	12 12
1	F	395/394 (100%)	360 (91%)	34 (9%)	1 (0%)	41 50
All	All	2310/2364 (98%)	2150 (93%)	129 (6%)	31 (1%)	12 12

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	SER
1	B	13	GLN
1	B	224	GLU
1	B	234	LEU
1	B	239	TRP

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Mol	Chain	Res	Type
1	B	321	SER
1	C	321	SER
1	D	20	PRO
1	D	22	LEU
1	D	72	LEU
1	D	313	GLY
1	D	321	SER
1	E	321	SER
1	B	226	GLU
1	A	1[A]	SER
1	A	1[B]	SER
1	C	221	SER
1	D	182	TRP
1	D	214	GLN
1	E	290	HIS
1	E	353	GLY
1	F	321	SER
1	B	18	VAL
1	B	221	SER
1	D	1	SER
1	D	339	ALA
1	E	224	GLU
1	D	314	ASP
1	B	188	PRO
1	E	110	GLY
1	D	10	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	307/305 (101%)	296 (96%)	11 (4%)	35 49
1	B	307/305 (101%)	281 (92%)	26 (8%)	10 13
1	C	305/305 (100%)	296 (97%)	9 (3%)	41 57
1	D	260/305 (85%)	226 (87%)	34 (13%)	4 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	306/305 (100%)	295 (96%)	11 (4%)	35 49
1	F	307/305 (101%)	296 (96%)	11 (4%)	35 49
All	All	1792/1830 (98%)	1690 (94%)	102 (6%)	20 28

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MET
1	A	78	ARG
1	A	83	GLU
1	A	139	ARG
1	A	153	TYR
1	A	157	ARG
1	A	224	GLU
1	A	226	GLU
1	A	286	TYR
1	A	344	ARG
1	A	379	ARG
1	B	0	MET
1	B	7	GLU
1	B	10	ILE
1	B	13	GLN
1	B	21	THR
1	B	24	MET
1	B	83	GLU
1	B	133	SER
1	B	139[A]	ARG
1	B	139[B]	ARG
1	B	140	LYS
1	B	155	GLU
1	B	157	ARG
1	B	159	LEU
1	B	193	ILE
1	B	198	PHE
1	B	216	LYS
1	B	218	LYS
1	B	229	ARG
1	B	239	TRP
1	B	260	LYS
1	B	286	TYR
1	B	316	PRO

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Mol	Chain	Res	Type
1	B	344	ARG
1	B	346	TYR
1	B	352	LEU
1	C	133	SER
1	C	152	TYR
1	C	162	SER
1	C	224	GLU
1	C	242	LEU
1	C	286	TYR
1	C	344	ARG
1	C	382	LYS
1	C	387	ASP
1	D	0	MET
1	D	3	TRP
1	D	6	TYR
1	D	8	ASN
1	D	10	ILE
1	D	18	VAL
1	D	22	LEU
1	D	60	GLU
1	D	72	LEU
1	D	78	ARG
1	D	106	GLN
1	D	144	ASP
1	D	153	TYR
1	D	157	ARG
1	D	165	ARG
1	D	180	ASP
1	D	183	ILE
1	D	187	ARG
1	D	203	CYS
1	D	204	LEU
1	D	205	THR
1	D	215	LYS
1	D	261	MET
1	D	286	TYR
1	D	293	ARG
1	D	299	LEU
1	D	314	ASP
1	D	320	ASP
1	D	321	SER
1	D	325	THR

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Mol	Chain	Res	Type
1	D	328	ASP
1	D	346	TYR
1	D	366	LEU
1	D	387	ASP
1	E	8	ASN
1	E	25	SER
1	E	78	ARG
1	E	111	ASP
1	E	139	ARG
1	E	152	TYR
1	E	226	GLU
1	E	246	SER
1	E	286	TYR
1	E	294	GLN
1	E	344	ARG
1	F	8	ASN
1	F	139	ARG
1	F	153	TYR
1	F	157	ARG
1	F	215	LYS
1	F	229	ARG
1	F	286	TYR
1	F	328	ASP
1	F	344	ARG
1	F	346	TYR
1	F	387	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

25 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	D	403	-	4,4,4	0.50	0	6,6,6	0.50	0
2	FMN	D	401	-	33,33,33	1.73	7 (21%)	48,50,50	1.89	7 (14%)
3	SO4	C	405	-	4,4,4	0.33	0	6,6,6	0.20	0
3	SO4	E	402	-	4,4,4	0.24	0	6,6,6	0.19	0
3	SO4	F	402	-	4,4,4	0.26	0	6,6,6	0.14	0
2	FMN	C	401	-	33,33,33	1.61	7 (21%)	48,50,50	1.66	9 (18%)
2	FMN	B	401	-	33,33,33	1.88	7 (21%)	48,50,50	1.25	4 (8%)
2	FMN	F	401	-	33,33,33	1.45	6 (18%)	48,50,50	1.43	9 (18%)
3	SO4	E	403	-	4,4,4	0.22	0	6,6,6	0.23	0
3	SO4	B	402	-	4,4,4	0.41	0	6,6,6	0.52	0
3	SO4	C	403	-	4,4,4	0.14	0	6,6,6	0.72	0
3	SO4	B	406	-	4,4,4	0.61	0	6,6,6	0.86	0
2	FMN	E	401	-	33,33,33	1.54	5 (15%)	48,50,50	1.45	11 (22%)
3	SO4	C	402	-	4,4,4	0.20	0	6,6,6	0.58	0
3	SO4	A	402	-	4,4,4	0.22	0	6,6,6	0.96	0
3	SO4	A	404[A]	-	4,4,4	0.30	0	6,6,6	0.38	0
3	SO4	C	404	-	4,4,4	0.50	0	6,6,6	0.54	0
3	SO4	F	403	-	4,4,4	0.22	0	6,6,6	0.47	0
3	SO4	A	405	-	4,4,4	0.37	0	6,6,6	0.29	0
2	FMN	A	401	-	33,33,33	1.80	10 (30%)	48,50,50	1.44	8 (16%)
3	SO4	A	403	-	4,4,4	0.47	0	6,6,6	0.89	0
3	SO4	B	403	-	4,4,4	0.41	0	6,6,6	0.58	0
3	SO4	B	404	-	4,4,4	0.25	0	6,6,6	0.43	0
3	SO4	B	405	-	4,4,4	0.22	0	6,6,6	0.11	0
3	SO4	D	402	-	4,4,4	0.30	0	6,6,6	0.69	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	D	401	-	-	5/18/18/18	0/3/3/3
2	FMN	C	401	-	-	1/18/18/18	0/3/3/3
2	FMN	B	401	-	-	2/18/18/18	0/3/3/3
2	FMN	F	401	-	-	4/18/18/18	0/3/3/3
2	FMN	A	401	-	-	5/18/18/18	0/3/3/3
2	FMN	E	401	-	-	1/18/18/18	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	FMN	C9A-C5A	5.49	1.50	1.41
2	B	401	FMN	C9A-C5A	5.42	1.49	1.41
2	F	401	FMN	C9A-C5A	4.93	1.49	1.41
2	C	401	FMN	C9A-C5A	4.34	1.48	1.41
2	B	401	FMN	C4A-N5	4.21	1.39	1.30
2	D	401	FMN	C9A-C5A	4.20	1.47	1.41
2	D	401	FMN	C8-C7	4.09	1.50	1.40
2	A	401	FMN	C9A-C5A	3.78	1.47	1.41
2	A	401	FMN	C6-C7	-3.62	1.34	1.39
2	E	401	FMN	C8-C7	3.60	1.49	1.40
2	B	401	FMN	C4-N3	-3.55	1.32	1.38
2	B	401	FMN	C8-C7	3.47	1.49	1.40
2	F	401	FMN	C8-C7	3.33	1.49	1.40
2	C	401	FMN	C4-N3	-3.12	1.33	1.38
2	B	401	FMN	C10-N1	2.87	1.39	1.33
2	C	401	FMN	O2-C2	2.81	1.29	1.24
2	B	401	FMN	C6-C7	-2.81	1.35	1.39
2	A	401	FMN	O2-C2	2.79	1.29	1.24
2	A	401	FMN	C9-C9A	-2.74	1.35	1.39
2	D	401	FMN	C10-N10	2.68	1.43	1.37
2	F	401	FMN	C4-N3	-2.67	1.33	1.38
2	D	401	FMN	O4-C4	2.66	1.28	1.23
2	A	401	FMN	C4-N3	-2.64	1.33	1.38
2	B	401	FMN	C9-C8	-2.62	1.36	1.39
2	D	401	FMN	C9A-N10	2.59	1.45	1.41
2	A	401	FMN	C1'-C2'	-2.58	1.49	1.52
2	D	401	FMN	C4A-N5	2.57	1.36	1.30
2	C	401	FMN	C6-C7	-2.46	1.36	1.39
2	C	401	FMN	C8-C7	2.41	1.46	1.40
2	C	401	FMN	C10-N10	2.33	1.42	1.37
2	A	401	FMN	C5'-C4'	2.32	1.55	1.51
2	E	401	FMN	C4-N3	-2.28	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	FMN	C5A-N5	-2.27	1.35	1.39
2	E	401	FMN	C10-N10	2.27	1.42	1.37
2	A	401	FMN	C2-N3	-2.24	1.34	1.39
2	F	401	FMN	C4A-N5	2.15	1.35	1.30
2	C	401	FMN	O4-C4	2.10	1.27	1.23
2	A	401	FMN	C4A-N5	2.06	1.35	1.30
2	A	401	FMN	C5A-N5	-2.05	1.35	1.39
2	F	401	FMN	C2-N3	-2.05	1.34	1.39
2	E	401	FMN	C5A-N5	-2.02	1.35	1.39
2	D	401	FMN	P-O5'	2.01	1.66	1.60

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	FMN	O4'-C4'-C5'	7.09	125.61	109.99
2	C	401	FMN	C9A-N10-C10	-5.04	113.06	120.75
2	D	401	FMN	O4'-C4'-C3'	-5.03	97.49	109.25
2	F	401	FMN	C9A-N10-C10	-4.05	114.57	120.75
2	A	401	FMN	C9A-C5A-N5	-3.76	118.47	122.45
2	C	401	FMN	C4A-C10-N10	3.73	121.83	116.48
2	E	401	FMN	C1'-C2'-C3'	3.54	119.26	109.66
2	F	401	FMN	C4-C4A-N5	3.40	122.90	118.21
2	A	401	FMN	C10-N1-C2	3.39	124.18	116.85
2	C	401	FMN	C10-N1-C2	3.38	124.17	116.85
2	D	401	FMN	C1'-C2'-C3'	3.33	118.70	109.66
2	D	401	FMN	O3'-C3'-C4'	-3.33	101.37	108.93
2	C	401	FMN	C4-C4A-N5	3.29	122.75	118.21
2	B	401	FMN	O4-C4-C4A	-3.19	118.10	126.53
2	E	401	FMN	O2-C2-N1	-3.16	116.55	121.80
2	A	401	FMN	C4A-C10-N1	-3.02	117.19	124.59
2	A	401	FMN	C9A-N10-C10	-3.02	116.15	120.75
2	E	401	FMN	C4A-C10-N1	-3.01	117.21	124.59
2	C	401	FMN	O5'-P-O1P	-3.00	98.34	106.44
2	A	401	FMN	O2'-C2'-C3'	2.92	116.09	109.25
2	E	401	FMN	C4A-C10-N10	2.83	120.53	116.48
2	B	401	FMN	C4A-C4-N3	2.82	120.42	113.25
2	E	401	FMN	C9A-N10-C10	-2.76	116.54	120.75
2	A	401	FMN	C4-C4A-N5	2.69	121.92	118.21
2	D	401	FMN	C4A-C10-N1	-2.66	118.06	124.59
2	F	401	FMN	C4A-C10-N10	2.63	120.25	116.48
2	B	401	FMN	C5A-C9A-N10	2.58	120.30	117.97
2	C	401	FMN	C10-C4A-N5	-2.53	119.63	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	FMN	C4'-C3'-C2'	-2.53	109.36	113.57
2	C	401	FMN	C4A-C10-N1	-2.51	118.45	124.59
2	E	401	FMN	C10-N1-C2	2.49	122.24	116.85
2	D	401	FMN	C5A-N5-C4A	2.44	122.03	118.09
2	F	401	FMN	C4A-C10-N1	-2.40	118.71	124.59
2	E	401	FMN	O4-C4-C4A	-2.38	120.25	126.53
2	E	401	FMN	C4-N3-C2	-2.37	121.44	125.64
2	F	401	FMN	C9A-C5A-N5	-2.35	119.96	122.45
2	E	401	FMN	O3P-P-O2P	2.23	116.17	107.80
2	A	401	FMN	C4A-C4-N3	2.21	118.87	113.25
2	F	401	FMN	C4A-C4-N3	2.21	118.87	113.25
2	F	401	FMN	O3P-P-O2P	2.18	115.97	107.80
2	E	401	FMN	C5A-C9A-N10	2.17	119.93	117.97
2	A	401	FMN	C10-C4A-N5	-2.16	120.39	124.81
2	F	401	FMN	C10-N1-C2	2.14	121.47	116.85
2	D	401	FMN	C10-C4A-N5	-2.13	120.47	124.81
2	E	401	FMN	C4A-C4-N3	2.10	118.60	113.25
2	C	401	FMN	O3P-P-O1P	2.08	118.92	110.83
2	F	401	FMN	C4-N3-C2	-2.04	122.02	125.64
2	B	401	FMN	O3P-P-O1P	2.01	118.68	110.83

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	FMN	C3'-C4'-C5'-O5'
2	D	401	FMN	O4'-C4'-C5'-O5'
2	D	401	FMN	C5'-O5'-P-O2P
2	D	401	FMN	C5'-O5'-P-O3P
2	A	401	FMN	O3'-C3'-C4'-C5'
2	A	401	FMN	C2'-C3'-C4'-O4'
2	F	401	FMN	C3'-C4'-C5'-O5'
2	A	401	FMN	O3'-C3'-C4'-O4'
2	D	401	FMN	C5'-O5'-P-O1P
2	F	401	FMN	O4'-C4'-C5'-O5'
2	A	401	FMN	C2'-C3'-C4'-C5'
2	C	401	FMN	C4'-C5'-O5'-P
2	B	401	FMN	C4'-C5'-O5'-P
2	A	401	FMN	C4'-C5'-O5'-P
2	E	401	FMN	C4'-C5'-O5'-P
2	F	401	FMN	C2'-C3'-C4'-O4'
2	F	401	FMN	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
2	B	401	FMN	O3'-C3'-C4'-O4'

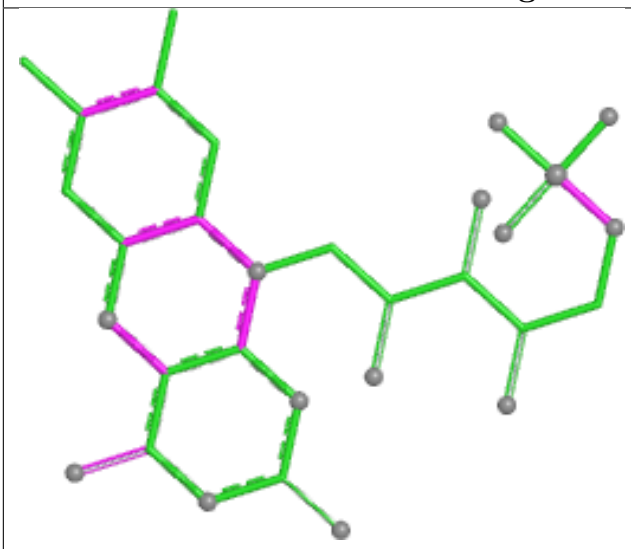
There are no ring outliers.

9 monomers are involved in 14 short contacts:

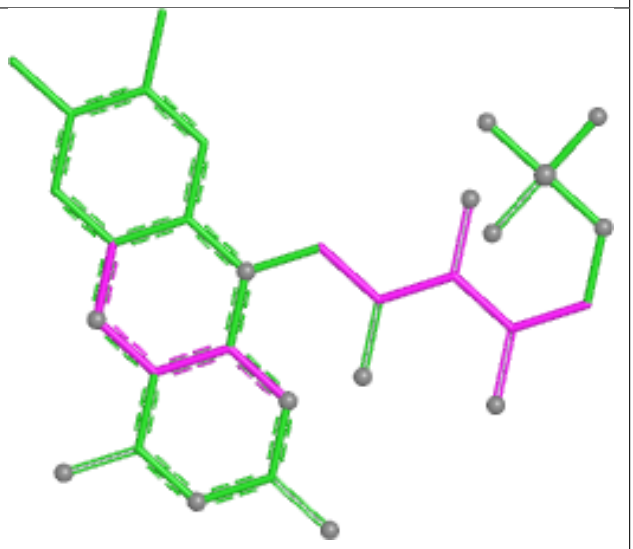
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	FMN	5	0
3	C	405	SO4	1	0
2	C	401	FMN	2	0
2	F	401	FMN	1	0
3	E	403	SO4	1	0
3	B	406	SO4	1	0
2	E	401	FMN	1	0
3	C	402	SO4	1	0
3	F	403	SO4	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

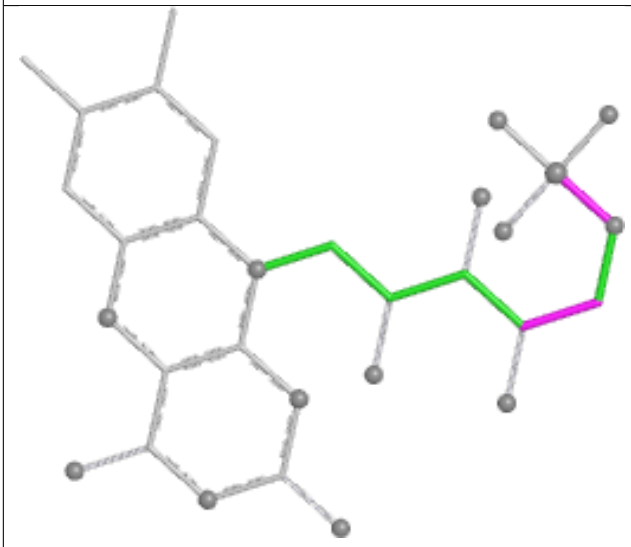
Ligand FMN D 401



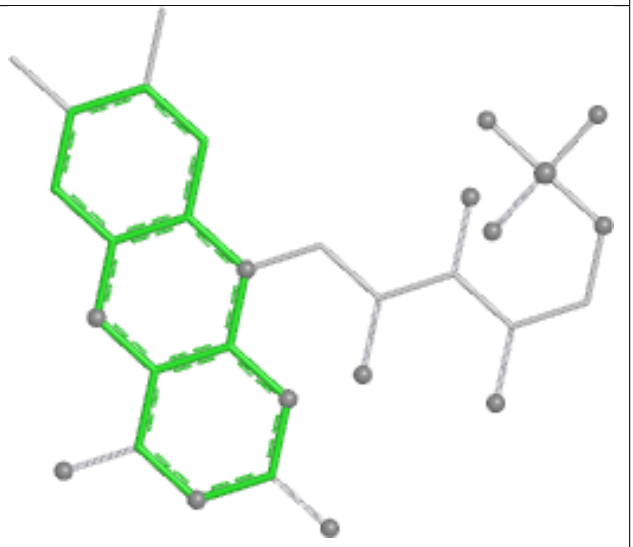
Bond lengths



Bond angles

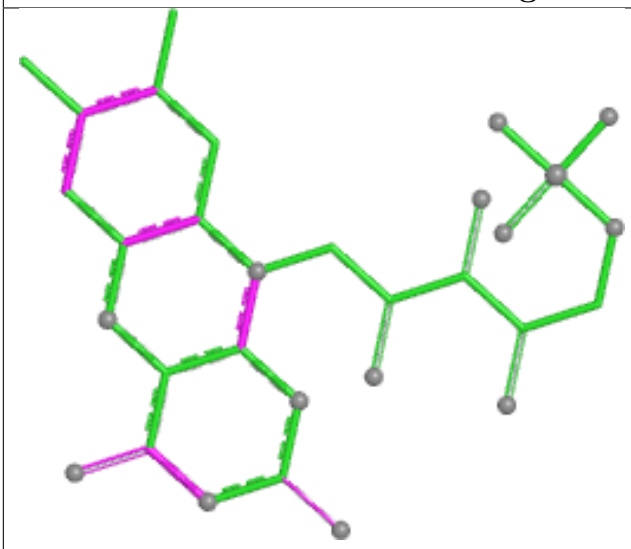


Torsions

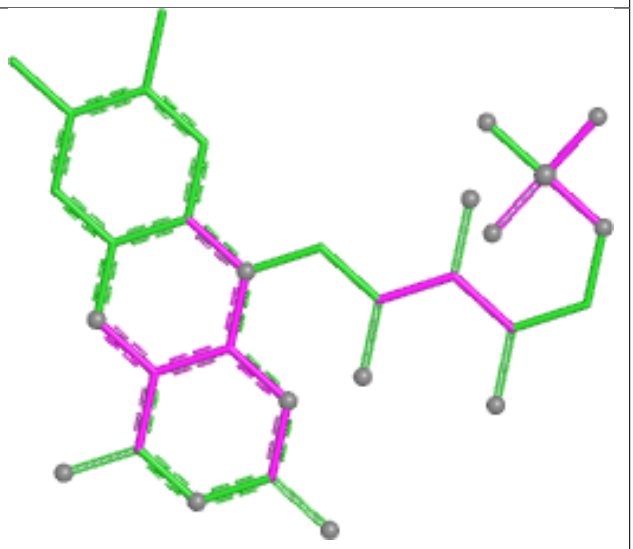


Rings

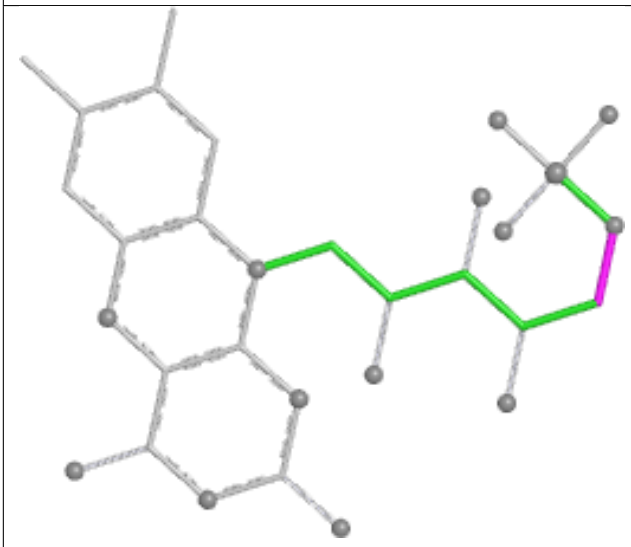
Ligand FMN C 401



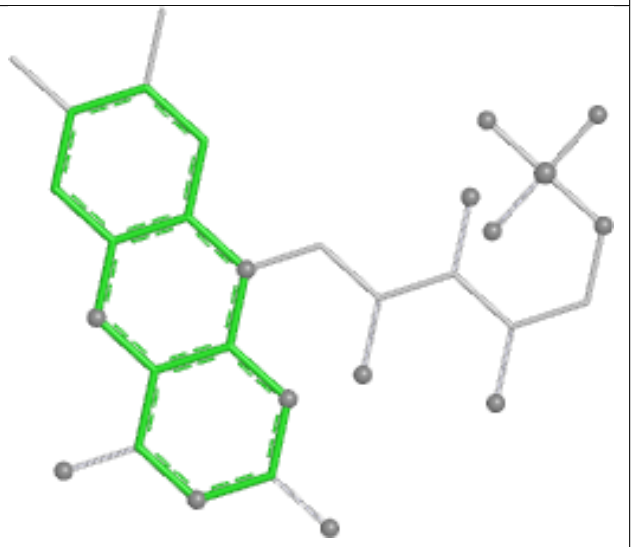
Bond lengths



Bond angles

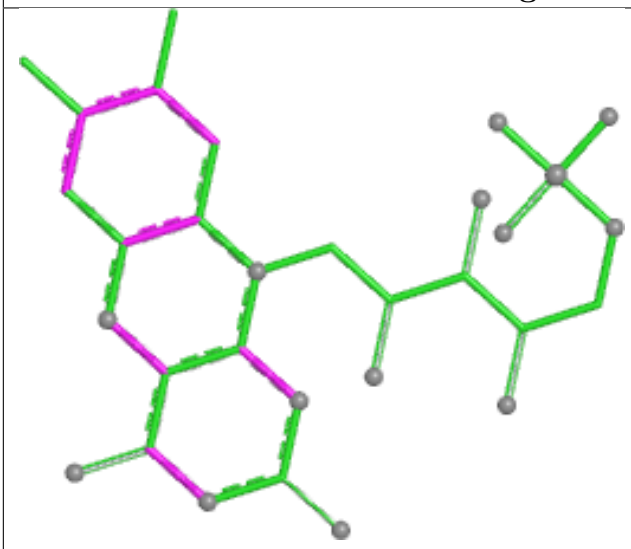


Torsions

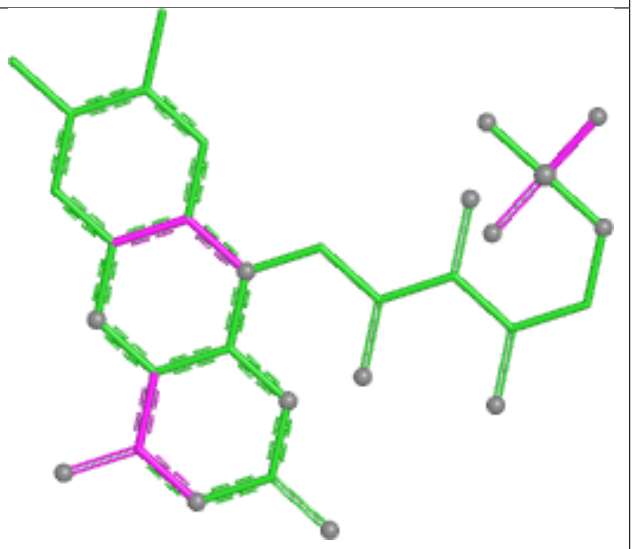


Rings

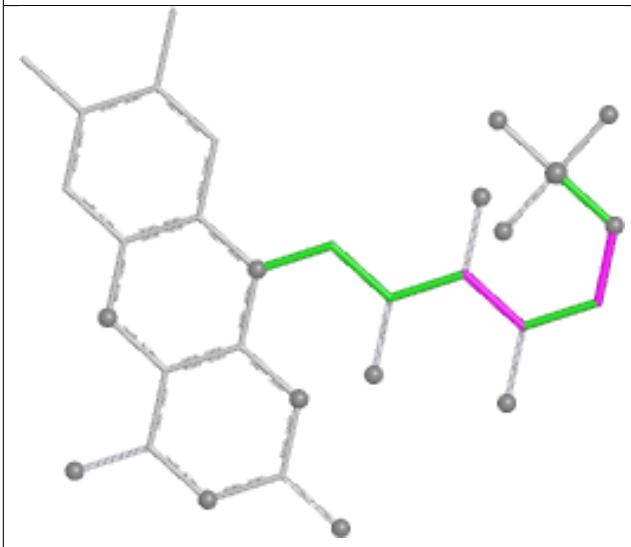
Ligand FMN B 401



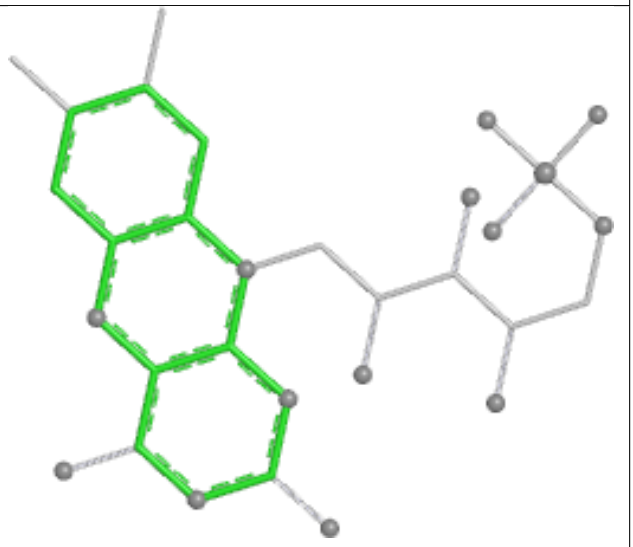
Bond lengths



Bond angles

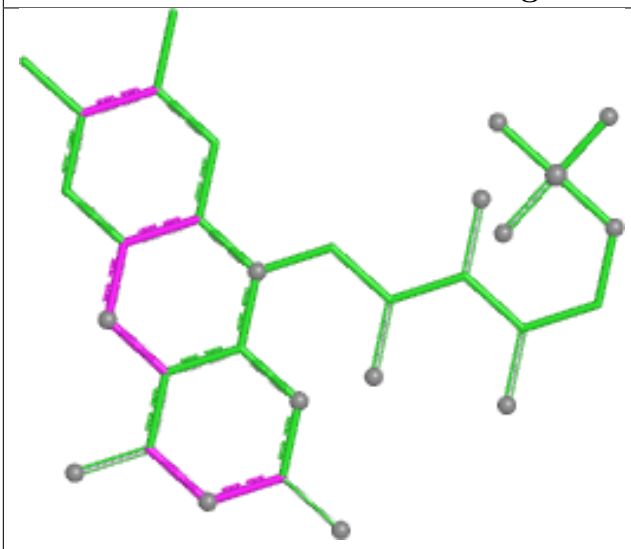


Torsions

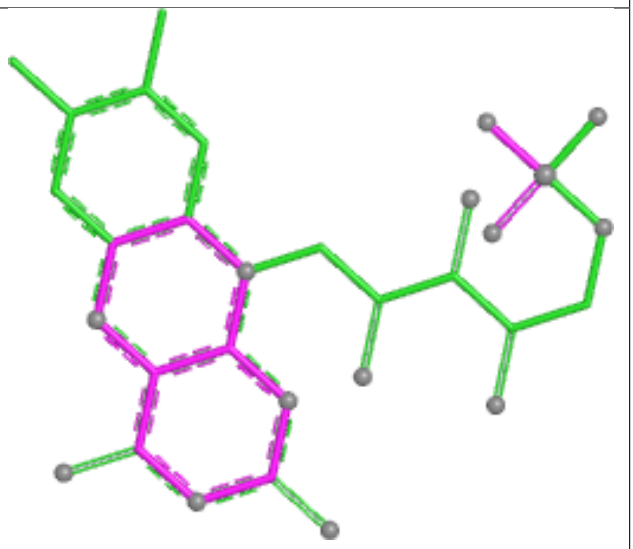


Rings

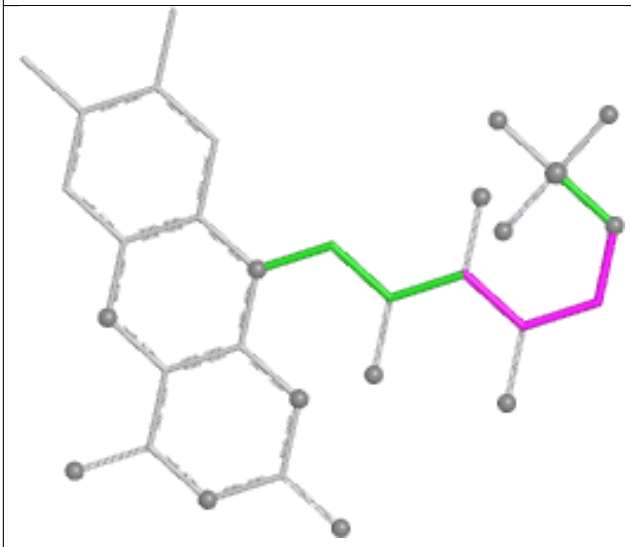
Ligand FMN F 401



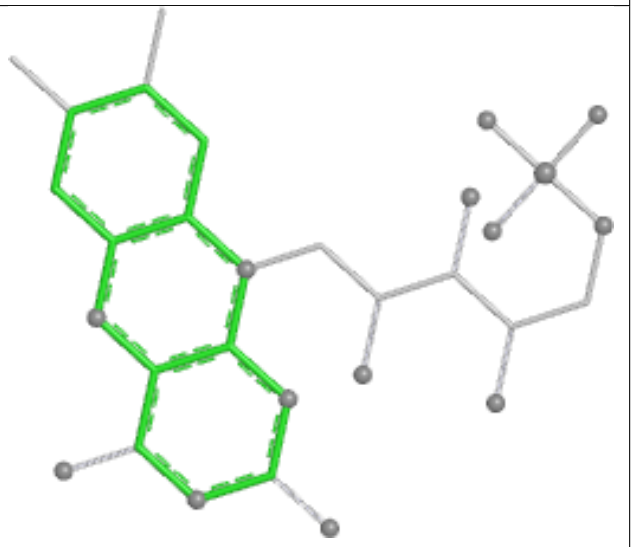
Bond lengths



Bond angles

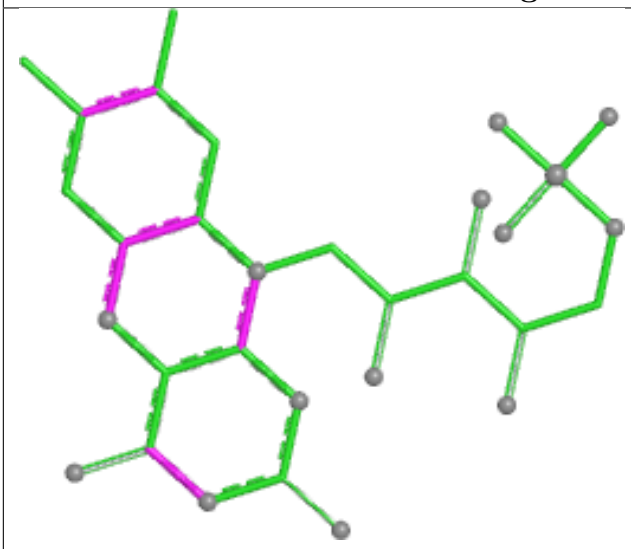


Torsions

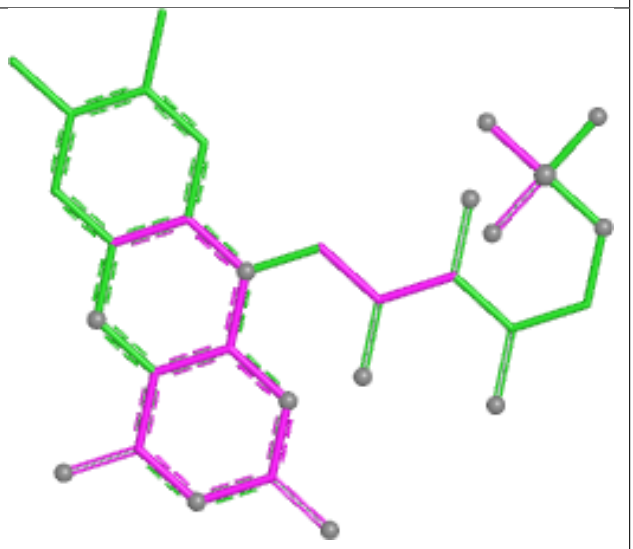


Rings

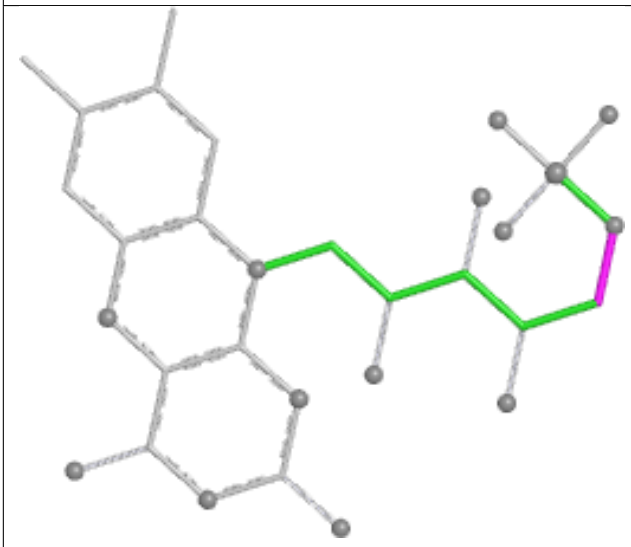
Ligand FMN E 401



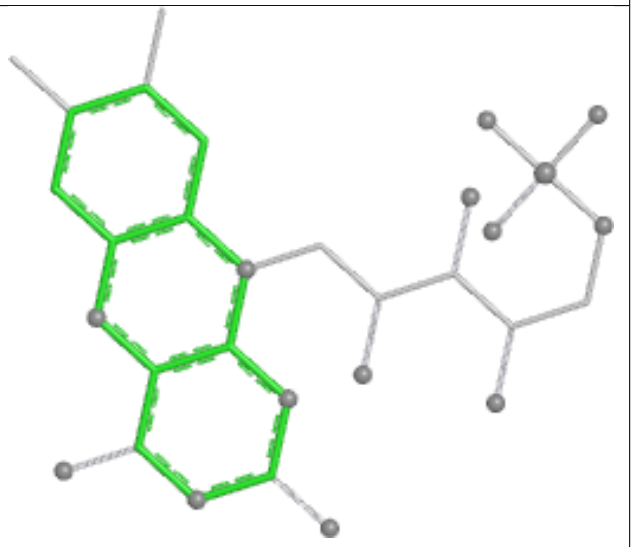
Bond lengths



Bond angles

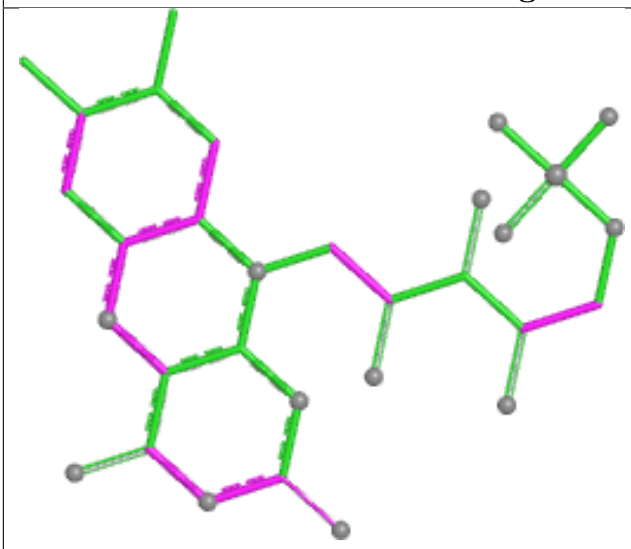


Torsions

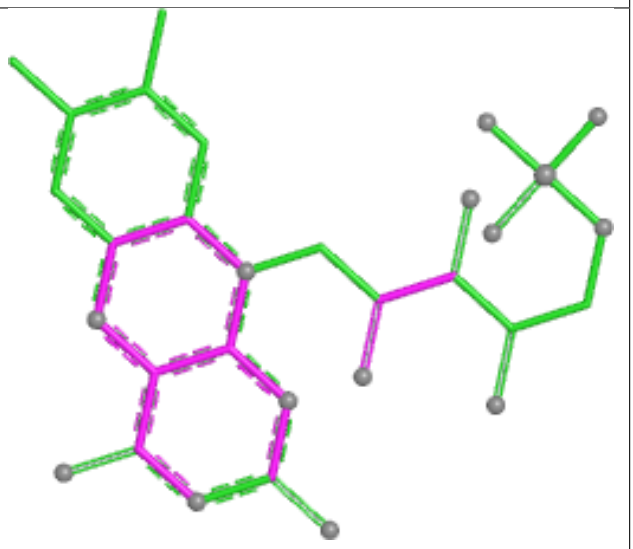


Rings

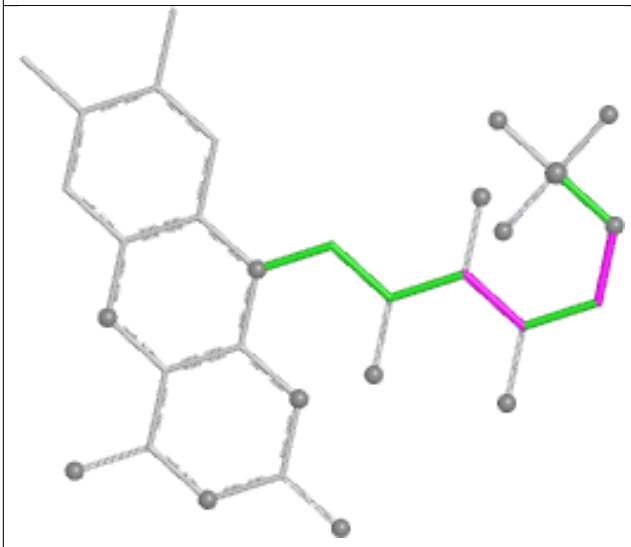
Ligand FMN A 401



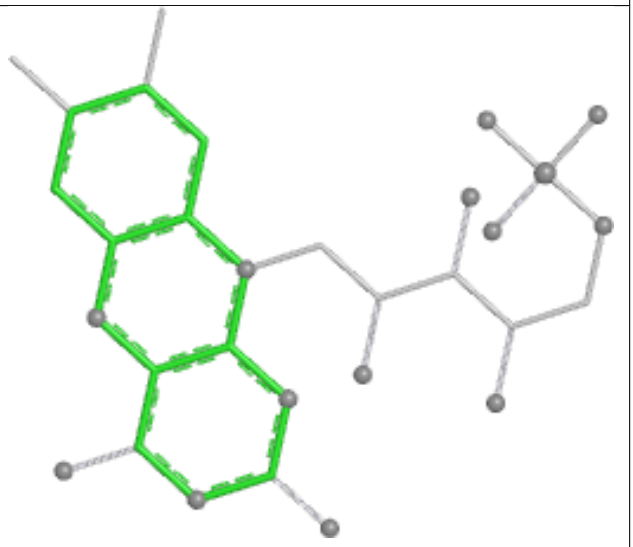
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	0.90	27 (6%) 16 22	14, 23, 36, 66	0
1	B	394/394 (100%)	1.37	77 (19%) 1 1	20, 34, 93, 156	0
1	C	394/394 (100%)	0.78	14 (3%) 42 49	20, 32, 49, 98	0
1	D	338/394 (85%)	2.79	210 (62%) 0 0	52, 72, 109, 173	0
1	E	393/394 (99%)	5.37	363 (92%) 0 0	84, 102, 146, 207	393 (100%)
1	F	393/394 (99%)	6.06	375 (95%) 0 0	102, 116, 166, 236	393 (100%)
All	All	2306/2364 (97%)	2.88	1066 (46%) 0 0	14, 59, 136, 236	786 (34%)

All (1066) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	138	ILE	45.0
1	E	227	GLY	23.1
1	F	108	GLY	22.6
1	E	254	TRP	19.8
1	F	23	PRO	18.0
1	E	351	ALA	17.9
1	F	219	ALA	17.8
1	F	223	VAL	17.5
1	F	226	GLU	16.2
1	E	223	VAL	16.0
1	F	122	GLY	15.6
1	F	204[A]	LEU	15.5
1	F	138	ILE	15.3
1	F	179	LEU	15.3
1	E	336	GLY	15.2
1	E	202	LEU	14.8
1	F	298	GLY	14.6
1	F	212	VAL	14.3
1	F	221	SER	14.1

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Mol	Chain	Res	Type	RSRZ
1	F	160	ALA	13.8
1	E	203	CYS	13.7
1	F	228	LEU	13.7
1	F	216	LYS	13.6
1	F	217	PHE	13.5
1	E	36	ALA	13.3
1	E	208[A]	VAL	13.1
1	F	239	TRP	13.1
1	F	57	ALA	12.7
1	F	137	ASP	12.3
1	E	364	SER	12.3
1	E	372	ILE	12.2
1	F	345	PRO	12.2
1	E	228	LEU	12.1
1	E	159	LEU	12.0
1	E	241	GLY	12.0
1	D	14	GLY	11.9
1	E	221	SER	11.9
1	E	255	VAL	11.8
1	F	213	PHE	11.8
1	F	49	SER	11.7
1	F	76	THR	11.6
1	F	112	ALA	11.6
1	E	91	ALA	11.6
1	F	315	THR	11.5
1	F	143	GLY	11.5
1	F	197	PRO	11.4
1	F	277	ALA	11.4
1	F	230	ASP	11.3
1	F	115	ALA	11.2
1	E	257	SER	11.2
1	F	19	ALA	11.1
1	F	269	GLN	11.1
1	F	227	GLY	11.1
1	F	164	ILE	11.0
1	E	264	ILE	11.0
1	E	333	LEU	10.9
1	E	235	ALA	10.9
1	F	107	ASP	10.9
1	E	277	ALA	10.8
1	F	75	ALA	10.8
1	F	69	PRO	10.7

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Mol	Chain	Res	Type	RSRZ
1	E	222	GLY	10.7
1	F	224	GLU	10.6
1	F	6	TYR	10.5
1	E	134	SER	10.5
1	E	7	GLU	10.5
1	F	378	TYR	10.4
1	B	228	LEU	10.4
1	E	346	TYR	10.4
1	E	142	ALA	10.4
1	F	308	VAL	10.4
1	F	244	GLY	10.3
1	F	84	LEU	10.3
1	F	126	ILE	10.3
1	F	210	ASP	10.2
1	F	220	HIS	10.2
1	E	252	ILE	10.2
1	E	213	PHE	10.1
1	F	92	PRO	10.1
1	F	99	GLY	10.1
1	F	225	ALA	10.1
1	E	240	HIS	10.0
1	E	308	VAL	9.9
1	E	217	PHE	9.9
1	F	149	PHE	9.9
1	E	156	ASP	9.9
1	D	21	THR	9.9
1	E	137	ASP	9.8
1	E	112	ALA	9.8
1	F	39	PRO	9.7
1	F	355	SER	9.7
1	E	358	ILE	9.7
1	F	94	PHE	9.7
1	F	361	VAL	9.6
1	F	282	VAL	9.6
1	F	250	GLU	9.6
1	E	246	SER	9.4
1	F	205	THR	9.4
1	F	159	LEU	9.4
1	E	176	VAL	9.4
1	E	158	ASP	9.4
1	E	151	LEU	9.3
1	E	363	ARG	9.3

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Mol	Chain	Res	Type	RSRZ
1	E	160	ALA	9.3
1	F	81	SER	9.3
1	F	139	ARG	9.3
1	F	352	LEU	9.3
1	E	113	ALA	9.3
1	E	212	VAL	9.2
1	F	365	LEU	9.2
1	E	45	VAL	9.2
1	F	372	ILE	9.2
1	F	290	HIS	9.2
1	F	265	LEU	9.1
1	E	23	PRO	9.1
1	E	347	ALA	9.1
1	F	254	TRP	9.1
1	B	231	ASN	9.0
1	E	183	ILE	9.0
1	E	74	ALA	9.0
1	F	215	LYS	9.0
1	E	234	LEU	8.9
1	E	37	LEU	8.9
1	D	279	ASP	8.9
1	F	154	PRO	8.9
1	F	186	TRP	8.9
1	F	93	MET	8.8
1	F	40	GLY	8.8
1	F	340	VAL	8.8
1	E	278	VAL	8.7
1	F	162	SER	8.7
1	E	103	LEU	8.7
1	D	274	ALA	8.7
1	F	259	THR	8.6
1	E	224	GLU	8.6
1	E	253	ASP	8.6
1	F	193	ILE	8.6
1	F	176	VAL	8.6
1	F	218	LYS	8.6
1	E	93	MET	8.5
1	E	114	SER	8.5
1	F	127	THR	8.5
1	E	312	SER	8.4
1	E	274	ALA	8.4
1	E	152	TYR	8.4

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Mol	Chain	Res	Type	RSRZ
1	E	141	HIS	8.4
1	E	218	LYS	8.4
1	F	22	LEU	8.4
1	F	371	LEU	8.3
1	B	225	ALA	8.3
1	F	274	ALA	8.2
1	E	207	TYR	8.2
1	F	207	TYR	8.2
1	F	117	ALA	8.2
1	F	264	ILE	8.1
1	F	181[A]	THR	8.1
1	E	206	ASN	8.1
1	F	148	TYR	8.1
1	E	263	VAL	8.0
1	F	242	LEU	8.0
1	B	198	PHE	8.0
1	F	42	LEU	8.0
1	B	236	ALA	8.0
1	F	38	PRO	8.0
1	F	377	GLY	8.0
1	F	286	TYR	8.0
1	F	161	GLU	8.0
1	E	165	ARG	8.0
1	F	163	PHE	8.0
1	F	130[A]	LEU	7.9
1	E	239	TRP	7.9
1	F	188	PRO	7.9
1	F	102	ALA	7.9
1	E	129	THR	7.9
1	F	248	THR	7.9
1	F	87	LYS	7.9
1	F	357	GLY	7.8
1	F	24	MET	7.8
1	E	281	GLY	7.7
1	E	350	ALA	7.7
1	E	115	ALA	7.7
1	F	184	PHE	7.7
1	E	161	GLU	7.7
1	D	164	ILE	7.6
1	E	191	LEU	7.6
1	E	211	PRO	7.6
1	F	214	GLN	7.6

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Mol	Chain	Res	Type	RSRZ
1	B	238	PHE	7.6
1	E	216	LYS	7.6
1	F	333	LEU	7.6
1	F	198	PHE	7.6
1	F	156	ASP	7.6
1	E	85	TRP	7.5
1	F	65	TRP	7.5
1	F	142	ALA	7.5
1	E	204	LEU	7.5
1	F	171	GLY	7.5
1	F	260	LYS	7.5
1	D	177	ILE	7.5
1	F	349	GLY	7.4
1	E	332	ALA	7.4
1	F	141	HIS	7.4
1	E	140	LYS	7.4
1	F	120	ARG	7.4
1	F	203	CYS	7.4
1	F	316	PRO	7.3
1	E	268	ILE	7.3
1	F	196	PHE	7.3
1	E	10	ILE	7.3
1	E	226	GLU	7.3
1	F	311	ALA	7.3
1	E	232	PRO	7.3
1	F	278	VAL	7.3
1	F	323	ILE	7.3
1	F	384	LEU	7.2
1	F	255	VAL	7.2
1	F	256	ARG	7.2
1	F	153	TYR	7.2
1	F	175	LEU	7.2
1	E	118	SER	7.2
1	D	301	ALA	7.2
1	F	267	GLY	7.2
1	E	41	VAL	7.1
1	E	294	GLN	7.1
1	F	91	ALA	7.1
1	F	350	ALA	7.1
1	F	281	GLY	7.1
1	E	367	ALA	7.1
1	F	113	ALA	7.1

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Mol	Chain	Res	Type	RSRZ
1	F	253	ASP	7.1
1	E	139	ARG	7.1
1	F	379	ARG	7.1
1	F	240	HIS	7.1
1	E	3	TRP	7.1
1	E	84	LEU	7.1
1	E	167	ALA	7.1
1	E	238	PHE	7.1
1	F	95	PHE	7.1
1	D	308	VAL	7.0
1	F	362	ALA	7.0
1	F	26	TYR	7.0
1	D	18	VAL	7.0
1	E	177	ILE	7.0
1	E	214	GLN	7.0
1	B	197	PRO	7.0
1	F	327	ALA	6.9
1	F	376	ASP	6.9
1	D	22	LEU	6.9
1	E	215	LYS	6.8
1	F	334	ALA	6.8
1	F	252	ILE	6.8
1	E	94	PHE	6.8
1	F	44	TYR	6.8
1	F	167	ALA	6.8
1	E	43	SER	6.8
1	E	210	ASP	6.8
1	F	235	ALA	6.8
1	B	217	PHE	6.7
1	F	231	ASN	6.7
1	F	125	TYR	6.7
1	F	104	CYS	6.7
1	F	97	PRO	6.7
1	E	102	ALA	6.7
1	D	15	LEU	6.7
1	D	6	TYR	6.6
1	F	45	VAL	6.6
1	F	183	ILE	6.6
1	D	20	PRO	6.6
1	E	258	ILE	6.6
1	E	31	ALA	6.6
1	F	172	TYR	6.6

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Mol	Chain	Res	Type	RSRZ
1	E	25	SER	6.5
1	E	199	LEU	6.5
1	F	335	MET	6.5
1	E	233	ARG	6.5
1	F	59	VAL	6.5
1	E	104	CYS	6.5
1	B	21	THR	6.5
1	F	152	TYR	6.5
1	E	135	LEU	6.5
1	D	121	THR	6.5
1	E	209	THR	6.4
1	D	75	ALA	6.4
1	F	268	ILE	6.4
1	F	229	ARG	6.4
1	E	335	MET	6.4
1	F	50	GLY	6.4
1	F	72	LEU	6.4
1	F	12	GLY	6.4
1	F	182	TRP	6.4
1	D	334	ALA	6.3
1	F	145	THR	6.3
1	D	91	ALA	6.3
1	F	271	PRO	6.3
1	E	145	THR	6.3
1	E	373	MET	6.3
1	E	310	LYS	6.2
1	D	151	LEU	6.2
1	F	246	SER	6.2
1	D	155	GLU	6.2
1	E	173	ASP	6.2
1	E	229	ARG	6.2
1	F	173	ASP	6.2
1	D	207	TYR	6.2
1	E	6	TYR	6.2
1	E	302	LEU	6.2
1	D	115	ALA	6.2
1	E	249	TRP	6.2
1	D	278	VAL	6.2
1	F	187[A]	ARG	6.2
1	D	0	MET	6.2
1	E	365	LEU	6.1
1	D	152	TYR	6.1

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Mol	Chain	Res	Type	RSRZ
1	F	208	VAL	6.1
1	F	318	LEU	6.1
1	F	222	GLY	6.1
1	E	97	PRO	6.1
1	E	87	LYS	6.1
1	E	22	LEU	6.1
1	F	353	GLY	6.1
1	F	380	ASN	6.1
1	E	121	THR	6.1
1	F	319	PHE	6.0
1	E	76	THR	6.0
1	E	219	ALA	6.0
1	E	261	MET	6.0
1	E	225	ALA	5.9
1	E	236	ALA	5.9
1	F	114	SER	5.9
1	E	201	GLY	5.9
1	F	383	GLU	5.9
1	F	209	THR	5.9
1	F	158	ASP	5.9
1	F	330	VAL	5.9
1	D	4	GLY	5.9
1	F	302	LEU	5.9
1	E	166	ARG	5.8
1	E	16	VAL	5.8
1	E	65	TRP	5.8
1	E	111	ASP	5.8
1	F	270	HIS	5.8
1	F	128	SER	5.8
1	F	73	MET	5.8
1	E	362	ALA	5.8
1	D	81	SER	5.8
1	E	366	LEU	5.8
1	E	384	LEU	5.8
1	F	343	GLY	5.8
1	F	177	ILE	5.8
1	E	318	LEU	5.8
1	D	184	PHE	5.7
1	E	116	GLN	5.7
1	F	85	TRP	5.7
1	E	256	ARG	5.7
1	E	286	TYR	5.7

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Mol	Chain	Res	Type	RSRZ
1	E	237	ASP	5.7
1	E	164	ILE	5.7
1	F	200	ARG	5.7
1	E	220	HIS	5.7
1	F	151	LEU	5.7
1	F	100	VAL	5.6
1	F	237	ASP	5.6
1	E	133	SER	5.6
1	E	282	VAL	5.6
1	E	290	HIS	5.6
1	E	100	VAL	5.6
1	E	175	LEU	5.6
1	F	4	GLY	5.6
1	C	0	MET	5.6
1	F	332	ALA	5.6
1	F	180	ASP	5.6
1	E	172	TYR	5.5
1	E	42	LEU	5.5
1	F	234	LEU	5.5
1	D	332	ALA	5.5
1	F	317	VAL	5.5
1	D	84	LEU	5.5
1	E	377	GLY	5.5
1	F	165	ARG	5.5
1	F	129	THR	5.5
1	F	68	MET	5.5
1	E	317	VAL	5.5
1	F	27	ALA	5.5
1	F	174	GLY	5.5
1	E	382	LYS	5.5
1	F	257	SER	5.5
1	F	74	ALA	5.5
1	E	389	LEU	5.4
1	B	234	LEU	5.4
1	F	310	LYS	5.4
1	F	98	ILE	5.4
1	F	9	GLU	5.4
1	C	225	ALA	5.4
1	F	386	ILE	5.4
1	E	259	THR	5.4
1	E	243	PHE	5.4
1	E	275	ARG	5.4

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Mol	Chain	Res	Type	RSRZ
1	F	285	ILE	5.3
1	E	205	THR	5.3
1	E	361	VAL	5.3
1	E	392	THR	5.3
1	E	271	PRO	5.3
1	E	179	LEU	5.3
1	E	248	THR	5.3
1	B	22	LEU	5.3
1	E	110	GLY	5.3
1	E	345	PRO	5.3
1	E	247	VAL	5.3
1	F	46	ALA	5.3
1	E	98	ILE	5.2
1	F	109	HIS	5.2
1	F	140	LYS	5.2
1	F	238	PHE	5.2
1	F	392	THR	5.2
1	F	1	SER	5.2
1	F	294	GLN	5.2
1	E	339	ALA	5.2
1	B	0	MET	5.2
1	F	37	LEU	5.2
1	F	373	MET	5.1
1	D	126	ILE	5.1
1	E	81	SER	5.1
1	F	303	ASP	5.1
1	E	390	ARG	5.1
1	F	276	ARG	5.1
1	D	374	ALA	5.1
1	E	170	ALA	5.1
1	E	29	TRP	5.1
1	E	83	GLU	5.1
1	F	80	LEU	5.1
1	E	82	VAL	5.1
1	F	291	GLY	5.1
1	F	304	CYS	5.1
1	E	319	PHE	5.1
1	E	334	ALA	5.1
1	E	117	ALA	5.0
1	F	309	VAL	5.0
1	D	122	GLY	5.0
1	E	380	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
1	E	28	ASP	5.0
1	D	163	PHE	5.0
1	F	131	ALA	5.0
1	F	13	GLN	5.0
1	E	61	ALA	5.0
1	F	194	SER	5.0
1	F	202	LEU	5.0
1	F	337	ALA	5.0
1	D	85	TRP	4.9
1	E	107	ASP	4.9
1	E	283	ASP	4.9
1	B	229	ARG	4.9
1	E	153	TYR	4.9
1	E	71	MET	4.9
1	E	162	SER	4.9
1	D	204	LEU	4.9
1	D	304	CYS	4.9
1	E	149	PHE	4.9
1	D	159	LEU	4.8
1	D	211	PRO	4.8
1	E	265	LEU	4.8
1	F	199	LEU	4.8
1	F	31	ALA	4.8
1	F	10	ILE	4.8
1	F	245	HIS	4.8
1	E	2	ASN	4.8
1	B	18	VAL	4.8
1	F	2	ASN	4.8
1	F	314	ASP	4.8
1	E	262	PRO	4.8
1	F	287	CYS	4.8
1	F	306	PRO	4.8
1	E	231	ASN	4.8
1	E	72	LEU	4.8
1	E	260	LYS	4.8
1	E	180	ASP	4.7
1	F	342	ILE	4.7
1	E	127	THR	4.7
1	E	80	LEU	4.7
1	F	11	TYR	4.7
1	F	247	VAL	4.7
1	F	385	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	120	ARG	4.7
1	D	16	VAL	4.7
1	E	20	PRO	4.7
1	E	230	ASP	4.7
1	D	94	PHE	4.7
1	E	307	GLU	4.7
1	E	13	GLN	4.7
1	E	330	VAL	4.6
1	E	26	TYR	4.6
1	B	16	VAL	4.6
1	B	193	ILE	4.6
1	E	144	ASP	4.6
1	D	49	SER	4.6
1	E	280[A]	SER	4.6
1	F	157	ARG	4.6
1	F	185	GLY	4.6
1	B	10	ILE	4.5
1	D	101	ILE	4.5
1	E	86	GLY	4.5
1	F	3	TRP	4.5
1	D	162	SER	4.5
1	E	128	SER	4.5
1	D	362	ALA	4.5
1	F	90	ALA	4.5
1	D	3	TRP	4.5
1	D	125	TYR	4.5
1	E	279	ASP	4.5
1	D	280	SER	4.4
1	E	321	SER	4.4
1	D	102	ALA	4.4
1	E	132	VAL	4.4
1	F	16	VAL	4.4
1	D	92	PRO	4.4
1	E	325	THR	4.4
1	F	66	GLY	4.4
1	D	90	ALA	4.4
1	E	357	GLY	4.4
1	D	160	ALA	4.4
1	F	263	VAL	4.4
1	D	127	THR	4.4
1	E	182	TRP	4.4
1	E	30	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	27	ALA	4.4
1	B	226	GLU	4.4
1	F	393	ARG	4.4
1	D	382	LYS	4.4
1	F	360	HIS	4.4
1	F	58	ASN	4.3
1	F	20	PRO	4.3
1	E	385	THR	4.3
1	D	167	ALA	4.3
1	E	184	PHE	4.3
1	D	42	LEU	4.3
1	B	17	GLY	4.3
1	E	163	PHE	4.3
1	F	119	ALA	4.3
1	D	158	ASP	4.3
1	E	370	ASP	4.3
1	E	186	TRP	4.3
1	F	364	SER	4.3
1	F	8	ASN	4.2
1	B	237	ASP	4.2
1	D	183	ILE	4.2
1	F	258	ILE	4.2
1	D	170	ALA	4.2
1	D	173	ASP	4.2
1	E	96	ALA	4.2
1	F	295	ALA	4.2
1	D	272	ASP	4.2
1	D	268	ILE	4.2
1	D	333	LEU	4.2
1	E	62	PHE	4.2
1	D	13	GLN	4.2
1	F	388	ALA	4.2
1	D	373	MET	4.2
1	D	385	THR	4.2
1	E	21	THR	4.2
1	E	155	GLU	4.2
1	E	124	PRO	4.2
1	F	211	PRO	4.2
1	F	329	VAL	4.2
1	F	351	ALA	4.2
1	D	298	GLY	4.2
1	F	144	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	37	LEU	4.1
1	F	135	LEU	4.1
1	E	378	TYR	4.1
1	E	329	VAL	4.1
1	F	356	LYS	4.1
1	E	311	ALA	4.1
1	E	323	ILE	4.1
1	B	240	HIS	4.1
1	B	15	LEU	4.1
1	F	320	ASP	4.1
1	B	207	TYR	4.1
1	E	69	PRO	4.1
1	F	86	GLY	4.1
1	D	19	ALA	4.1
1	F	18	VAL	4.1
1	F	367	ALA	4.1
1	E	77	GLU	4.1
1	E	304	CYS	4.1
1	F	272	ASP	4.1
1	F	110	GLY	4.1
1	A	29[A]	TRP	4.1
1	E	18	VAL	4.1
1	E	38	PRO	4.1
1	F	17	GLY	4.1
1	F	233	ARG	4.1
1	F	293	ARG	4.1
1	F	206	ASN	4.1
1	F	29	TRP	4.0
1	D	154	PRO	4.0
1	E	316	PRO	4.0
1	D	353	GLY	4.0
1	F	89	TRP	4.0
1	E	305	LEU	4.0
1	D	275	ARG	4.0
1	D	327	ALA	4.0
1	E	11	TYR	4.0
1	D	208	VAL	4.0
1	E	287	CYS	4.0
1	F	15	LEU	4.0
1	E	270	HIS	4.0
1	E	136	GLU	4.0
1	D	182	TRP	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	118	SER	4.0
1	F	375	VAL	4.0
1	E	353	GLY	3.9
1	F	78	ARG	3.9
1	F	283	ASP	3.9
1	D	282	VAL	3.9
1	E	59	VAL	3.9
1	F	51	ASP	3.9
1	F	169	GLU	3.9
1	B	190	ASP	3.9
1	B	211	PRO	3.9
1	E	315	THR	3.9
1	E	293	ARG	3.9
1	E	309	VAL	3.9
1	F	236	ALA	3.9
1	F	381	LEU	3.9
1	E	168	GLU	3.9
1	D	212	VAL	3.9
1	B	188	PRO	3.8
1	D	104	CYS	3.8
1	F	347	ALA	3.8
1	F	150	GLN	3.8
1	E	328	ASP	3.8
1	D	386	ILE	3.8
1	F	348	TRP	3.8
1	E	147	ALA	3.8
1	D	17	GLY	3.8
1	F	305	LEU	3.8
1	E	51	ASP	3.8
1	F	35	GLN	3.8
1	E	19	ALA	3.8
1	F	118	SER	3.8
1	D	376	ASP	3.8
1	E	89	TRP	3.8
1	E	200	ARG	3.8
1	F	321	SER	3.8
1	F	136	GLU	3.7
1	E	130	LEU	3.7
1	F	382	LYS	3.7
1	D	27	ALA	3.7
1	F	36	ALA	3.7
1	D	100	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	325	THR	3.7
1	F	331	LYS	3.7
1	F	289	ASN	3.7
1	F	288	SER	3.7
1	D	286	TYR	3.7
1	E	349	GLY	3.7
1	D	149	PHE	3.7
1	E	101	ILE	3.7
1	F	338	SER	3.7
1	E	340[A]	VAL	3.7
1	F	262	PRO	3.7
1	E	12	GLY	3.7
1	F	48	GLY	3.7
1	F	195	ASN	3.7
1	F	280	SER	3.7
1	F	326	GLY	3.7
1	F	339	ALA	3.7
1	E	150	GLN	3.7
1	D	381	LEU	3.6
1	F	170	ALA	3.6
1	D	11	TYR	3.6
1	E	24	MET	3.6
1	E	187	ARG	3.6
1	D	114	SER	3.6
1	E	360	HIS	3.6
1	D	267	GLY	3.6
1	D	156	ASP	3.6
1	F	307	GLU	3.6
1	D	349	GLY	3.6
1	F	7	GLU	3.6
1	E	338	SER	3.6
1	F	14	GLY	3.6
1	E	383	GLU	3.6
1	D	148	TYR	3.6
1	F	52	GLU	3.6
1	F	358	ILE	3.6
1	D	132	VAL	3.6
1	F	103	LEU	3.6
1	D	153	TYR	3.6
1	F	243	PHE	3.5
1	D	82	VAL	3.5
1	D	38	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	196	PHE	3.5
1	E	342	ILE	3.5
1	F	266	LYS	3.5
1	E	53	HIS	3.5
1	E	66	GLY	3.5
1	D	309	VAL	3.5
1	D	283	ASP	3.5
1	D	64	HIS	3.5
1	E	143	GLY	3.5
1	E	79	ASP	3.5
1	F	25	SER	3.5
1	D	138	ILE	3.4
1	E	193	ILE	3.4
1	E	299	LEU	3.4
1	E	197	PRO	3.4
1	D	270	HIS	3.4
1	E	381	LEU	3.4
1	F	299	LEU	3.4
1	E	251	ASP	3.4
1	E	272	ASP	3.4
1	D	302	LEU	3.4
1	F	178	THR	3.4
1	E	295	ALA	3.4
1	F	60	GLU	3.4
1	D	172	TYR	3.4
1	D	305	LEU	3.4
1	E	119	ALA	3.4
1	E	327	ALA	3.4
1	C	29[A]	TRP	3.4
1	C	220	HIS	3.4
1	E	64	HIS	3.4
1	F	32	HIS	3.4
1	F	79	ASP	3.4
1	F	297	GLY	3.3
1	F	34	GLN	3.3
1	D	131	ALA	3.3
1	D	142	ALA	3.3
1	E	90	ALA	3.3
1	F	190	ASP	3.3
1	F	166	ARG	3.3
1	F	21	THR	3.3
1	E	314	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	68	MET	3.3
1	F	275	ARG	3.3
1	E	267	GLY	3.3
1	D	365	LEU	3.3
1	E	188	PRO	3.3
1	D	315	THR	3.3
1	A	65	TRP	3.2
1	B	232	PRO	3.2
1	E	15	LEU	3.2
1	B	200	ARG	3.2
1	F	389	LEU	3.2
1	D	323	ILE	3.2
1	E	198	PHE	3.2
1	E	297	GLY	3.2
1	F	28	ASP	3.2
1	E	379	ARG	3.2
1	D	261	MET	3.2
1	D	318	LEU	3.2
1	F	346	TYR	3.2
1	B	192	THR	3.2
1	D	54	THR	3.2
1	F	105	ALA	3.2
1	B	230	ASP	3.2
1	D	176	VAL	3.2
1	D	276	ARG	3.2
1	D	96	ALA	3.2
1	E	17	GLY	3.2
1	E	40	GLY	3.2
1	E	48	GLY	3.2
1	E	284	GLY	3.2
1	D	76	THR	3.2
1	D	325	THR	3.2
1	E	356	LYS	3.2
1	F	55	GLN	3.2
1	D	321	SER	3.2
1	F	146	PRO	3.1
1	F	232	PRO	3.1
1	D	299	LEU	3.1
1	D	135	LEU	3.1
1	D	166	ARG	3.1
1	E	52	GLU	3.1
1	F	249	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	20	PRO	3.1
1	D	351	ALA	3.1
1	E	368	GLU	3.1
1	E	34	GLN	3.1
1	E	126	ILE	3.1
1	D	105	ALA	3.1
1	C	255	VAL	3.1
1	A	0	MET	3.1
1	D	306	PRO	3.1
1	B	323[A]	ILE	3.1
1	B	25	SER	3.0
1	D	80	LEU	3.0
1	D	5	ASP	3.0
1	D	144	ASP	3.0
1	F	116	GLN	3.0
1	D	181	THR	3.0
1	E	298	GLY	3.0
1	F	322	GLY	3.0
1	D	88	THR	3.0
1	D	370	ASP	3.0
1	F	279	ASP	3.0
1	B	8	ASN	3.0
1	B	195	ASN	3.0
1	B	233	ARG	3.0
1	D	213	PHE	3.0
1	D	281	GLY	3.0
1	F	241	GLY	3.0
1	F	292	GLY	3.0
1	D	111	ASP	3.0
1	F	251	ASP	3.0
1	E	73	MET	3.0
1	E	8	ASN	3.0
1	D	264	ILE	3.0
1	F	30	GLU	3.0
1	E	245	HIS	3.0
1	D	277	ALA	3.0
1	E	75	ALA	3.0
1	F	106	GLN	3.0
1	D	123	VAL	3.0
1	D	338	SER	2.9
1	E	291	GLY	2.9
1	F	83	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	377	GLY	2.9
1	D	1	SER	2.9
1	E	49	SER	2.9
1	D	33	ALA	2.9
1	D	311	ALA	2.9
1	D	313	GLY	2.9
1	E	196	PHE	2.9
1	F	132	VAL	2.9
1	A	1[A]	SER	2.9
1	F	370	ASP	2.9
1	D	179	LEU	2.9
1	D	186	TRP	2.9
1	F	64	HIS	2.9
1	E	1	SER	2.9
1	B	299	LEU	2.9
1	D	31	ALA	2.9
1	F	67	LEU	2.9
1	F	301	ALA	2.9
1	B	11	TYR	2.9
1	F	88	THR	2.8
1	B	305	LEU	2.8
1	F	300	PRO	2.8
1	E	194	SER	2.8
1	E	355	SER	2.8
1	D	67	LEU	2.8
1	D	369	ALA	2.8
1	F	133	SER	2.8
1	D	178	THR	2.8
1	C	223	VAL	2.8
1	E	375	VAL	2.8
1	E	300	PRO	2.8
1	A	304	CYS	2.8
1	E	99	GLY	2.8
1	E	348	TRP	2.8
1	B	219	ALA	2.8
1	F	313	GLY	2.8
1	F	344	ARG	2.8
1	E	108	GLY	2.8
1	F	121	THR	2.8
1	B	35	GLN	2.8
1	E	292	GLY	2.7
1	F	56	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	306	PRO	2.7
1	B	351	ALA	2.7
1	E	322	GLY	2.7
1	F	62	PHE	2.7
1	B	389	LEU	2.7
1	D	150	GLN	2.7
1	F	82	VAL	2.7
1	D	352	LEU	2.7
1	F	191	LEU	2.7
1	F	71	MET	2.7
1	E	32	HIS	2.7
1	B	302	LEU	2.7
1	B	384	LEU	2.7
1	E	303	ASP	2.7
1	D	140	LYS	2.7
1	D	206	ASN	2.7
1	B	212	VAL	2.7
1	E	67	LEU	2.7
1	A	322	GLY	2.7
1	B	189	ARG	2.7
1	D	316	PRO	2.7
1	D	147	ALA	2.7
1	E	296	ASN	2.7
1	F	53	HIS	2.7
1	B	67	LEU	2.7
1	D	161	GLU	2.6
1	E	376	ASP	2.6
1	F	61	ALA	2.6
1	B	322	GLY	2.6
1	D	66	GLY	2.6
1	D	262	PRO	2.6
1	B	353	GLY	2.6
1	D	45	VAL	2.6
1	D	113	ALA	2.6
1	F	168	GLU	2.6
1	D	175	LEU	2.6
1	E	242	LEU	2.6
1	D	136	GLU	2.6
1	D	53	HIS	2.6
1	D	350	ALA	2.6
1	F	33	ALA	2.6
1	D	361	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	92	PRO	2.6
1	D	354	GLY	2.6
1	D	379	ARG	2.6
1	E	331	LYS	2.6
1	E	154	PRO	2.6
1	D	32	HIS	2.6
1	F	387	ASP	2.6
1	E	388	ALA	2.6
1	F	324	ARG	2.5
1	A	203	CYS	2.5
1	D	103	LEU	2.5
1	D	61	ALA	2.5
1	E	285	ILE	2.5
1	B	199	LEU	2.5
1	D	210	ASP	2.5
1	D	141	HIS	2.5
1	D	335	MET	2.5
1	E	57	ALA	2.5
1	F	96	ALA	2.5
1	E	269	GLN	2.5
1	D	171	GLY	2.5
1	D	384	LEU	2.5
1	A	45	VAL	2.5
1	F	41	VAL	2.5
1	B	203	CYS	2.5
1	E	33	ALA	2.5
1	D	28	ASP	2.5
1	E	386	ILE	2.5
1	D	290	HIS	2.5
1	F	134	SER	2.5
1	D	39	PRO	2.5
1	E	14	GLY	2.5
1	B	13	GLN	2.5
1	E	39	PRO	2.5
1	E	181	THR	2.5
1	D	77	GLU	2.5
1	D	383	GLU	2.4
1	D	29	TRP	2.4
1	A	229	ARG	2.4
1	E	9	GLU	2.4
1	B	325	THR	2.4
1	E	44	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	387	ASP	2.4
1	E	352	LEU	2.4
1	E	371	LEU	2.4
1	D	12	GLY	2.4
1	F	336	GLY	2.4
1	F	341	GLY	2.4
1	E	148	TYR	2.4
1	B	335	MET	2.4
1	D	112	ALA	2.4
1	A	392	THR	2.4
1	B	309	VAL	2.4
1	F	296	ASN	2.4
1	D	51	ASP	2.4
1	A	388	ALA	2.4
1	B	300	PRO	2.4
1	E	68	MET	2.4
1	F	354	GLY	2.3
1	B	186	TRP	2.3
1	B	242	LEU	2.3
1	B	243	PHE	2.3
1	D	185	GLY	2.3
1	B	102	ALA	2.3
1	B	202	LEU	2.3
1	B	235	ALA	2.3
1	E	374	ALA	2.3
1	B	205	THR	2.3
1	B	224	GLU	2.3
1	F	359	GLU	2.3
1	E	326	GLY	2.3
1	F	273	ASP	2.3
1	A	305	LEU	2.3
1	B	54	THR	2.3
1	B	221	SER	2.3
1	E	106	GLN	2.3
1	B	65	TRP	2.3
1	A	309	VAL	2.3
1	B	223	VAL	2.3
1	E	391	PRO	2.3
1	F	5	ASP	2.3
1	E	131	ALA	2.3
1	D	375	VAL	2.3
1	D	320	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	350	ALA	2.3
1	A	42	LEU	2.2
1	D	129	THR	2.2
1	A	193	ILE	2.2
1	E	169	GLU	2.2
1	D	336	GLY	2.2
1	C	260	LYS	2.2
1	D	312	SER	2.2
1	A	61	ALA	2.2
1	D	117	ALA	2.2
1	E	393	ARG	2.2
1	F	391	PRO	2.2
1	A	375	VAL	2.2
1	E	341	GLY	2.2
1	B	19	ALA	2.2
1	E	301	ALA	2.2
1	A	371	LEU	2.2
1	A	389	LEU	2.2
1	C	37	LEU	2.2
1	E	123	VAL	2.2
1	A	62	PHE	2.2
1	D	303	ASP	2.2
1	D	106	GLN	2.2
1	D	392	THR	2.2
1	A	10	ILE	2.2
1	F	101	ILE	2.2
1	B	306	PRO	2.2
1	D	145	THR	2.2
1	D	388	ALA	2.2
1	A	98	ILE	2.2
1	A	384	LEU	2.2
1	E	5	ASP	2.2
1	A	329	VAL	2.1
1	C	204	LEU	2.1
1	C	353	GLY	2.1
1	E	343	GLY	2.1
1	F	77	GLU	2.1
1	E	63	LYS	2.1
1	D	372	ILE	2.1
1	A	300	PRO	2.1
1	D	389	LEU	2.1
1	E	289	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	317	VAL	2.1
1	E	266	LYS	2.1
1	D	62	PHE	2.1
1	E	58	ASN	2.1
1	E	70	ARG	2.1
1	D	287	CYS	2.1
1	D	169	GLU	2.1
1	E	324	ARG	2.1
1	B	14	GLY	2.1
1	C	227	GLY	2.1
1	E	47	GLY	2.1
1	B	169	GLU	2.1
1	F	390	ARG	2.1
1	E	46	ALA	2.1
1	B	191	LEU	2.1
1	E	359	GLU	2.1
1	D	24[A]	MET	2.1
1	A	348	TRP	2.1
1	C	59	VAL	2.1
1	C	84	LEU	2.0
1	F	63	LYS	2.0
1	D	2	ASN	2.0
1	E	174	GLY	2.0
1	F	374	ALA	2.0
1	D	34	GLN	2.0
1	E	273	ASP	2.0
1	F	328	ASP	2.0
1	E	157	ARG	2.0
1	A	299	LEU	2.0
1	B	371	LEU	2.0
1	C	302	LEU	2.0
1	F	261	MET	2.0
1	E	60	GLU	2.0
1	D	205	THR	2.0
1	D	288	SER	2.0
1	D	310	LYS	2.0
1	D	330	VAL	2.0
1	D	189	ARG	2.0
1	E	78	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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.

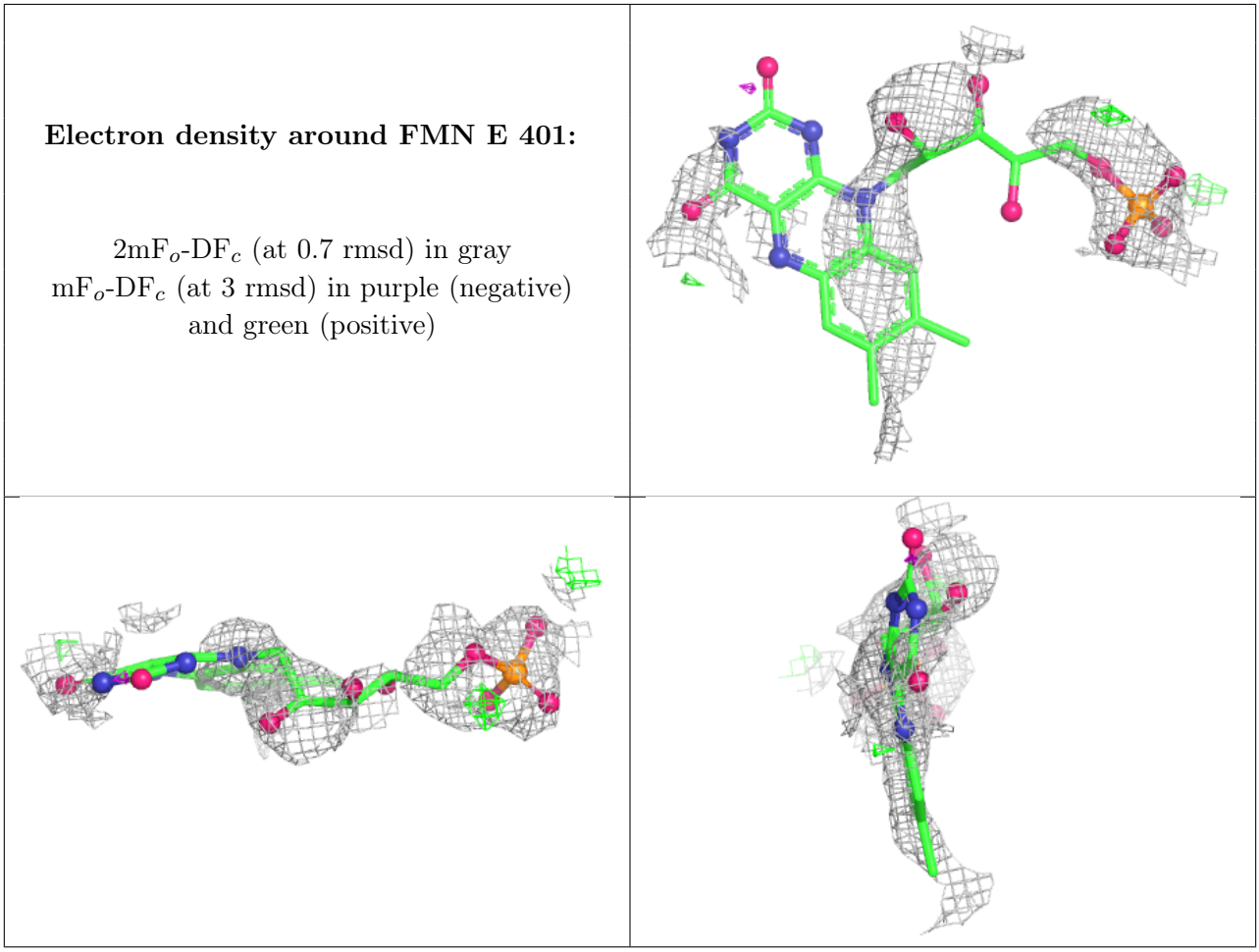
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FMN	E	401	31/31	0.48	0.48	65,86,106,116	31
3	SO4	F	402	5/5	0.61	0.50	83,86,113,120	5
3	SO4	E	402	5/5	0.68	0.39	110,112,131,140	5
2	FMN	F	401	31/31	0.68	0.32	68,92,102,107	31
3	SO4	B	404	5/5	0.73	0.44	53,61,74,83	5
3	SO4	B	406	5/5	0.74	0.17	44,45,52,73	0
3	SO4	C	405	5/5	0.74	0.29	32,43,47,64	5
2	FMN	D	401	31/31	0.77	0.24	26,42,52,57	0
3	SO4	A	404[A]	5/5	0.81	0.36	30,33,62,68	5
3	SO4	E	403	5/5	0.85	0.21	85,89,116,119	5
2	FMN	A	401	31/31	0.91	0.21	9,15,21,22	0
2	FMN	B	401	31/31	0.91	0.20	12,22,29,35	0
2	FMN	C	401	31/31	0.92	0.18	16,24,32,34	0
3	SO4	F	403	5/5	0.92	0.17	48,65,69,74	5
3	SO4	A	405	5/5	0.93	0.19	60,62,64,74	5
3	SO4	B	405	5/5	0.94	0.15	94,98,110,115	0
3	SO4	D	403	5/5	0.94	0.14	39,54,69,72	0
3	SO4	C	404	5/5	0.96	0.20	52,55,60,70	0
3	SO4	D	402	5/5	0.97	0.23	45,47,52,56	0
3	SO4	A	402	5/5	0.98	0.18	28,33,40,40	0
3	SO4	C	402	5/5	0.99	0.21	27,32,39,53	0
3	SO4	C	403	5/5	0.99	0.17	33,34,50,51	0
3	SO4	A	403	5/5	0.99	0.20	24,25,27,27	0
3	SO4	B	402	5/5	0.99	0.17	33,40,47,49	0
3	SO4	B	403	5/5	0.99	0.18	29,33,38,39	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.

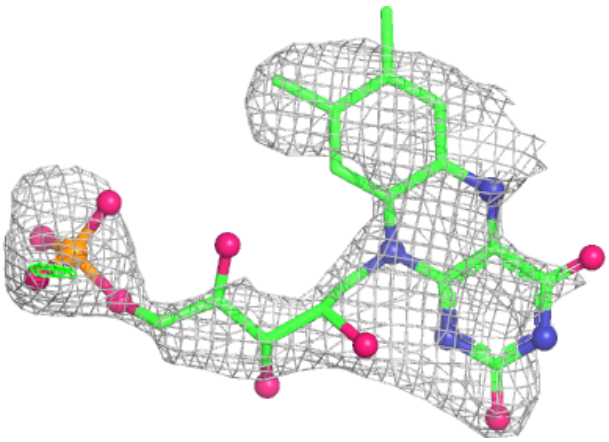
Electron density around FMN E 401:

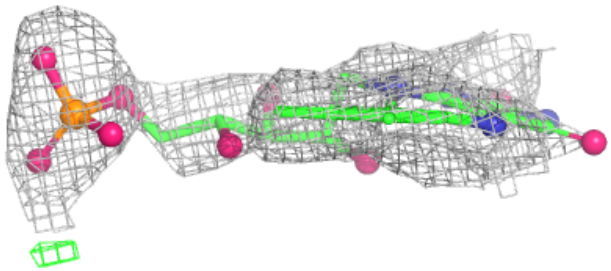
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

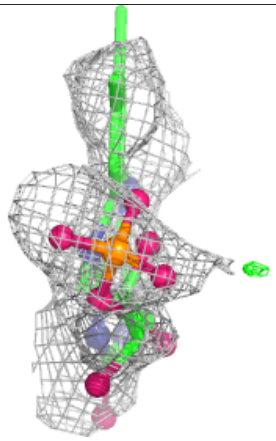


Electron density around FMN F 401:

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

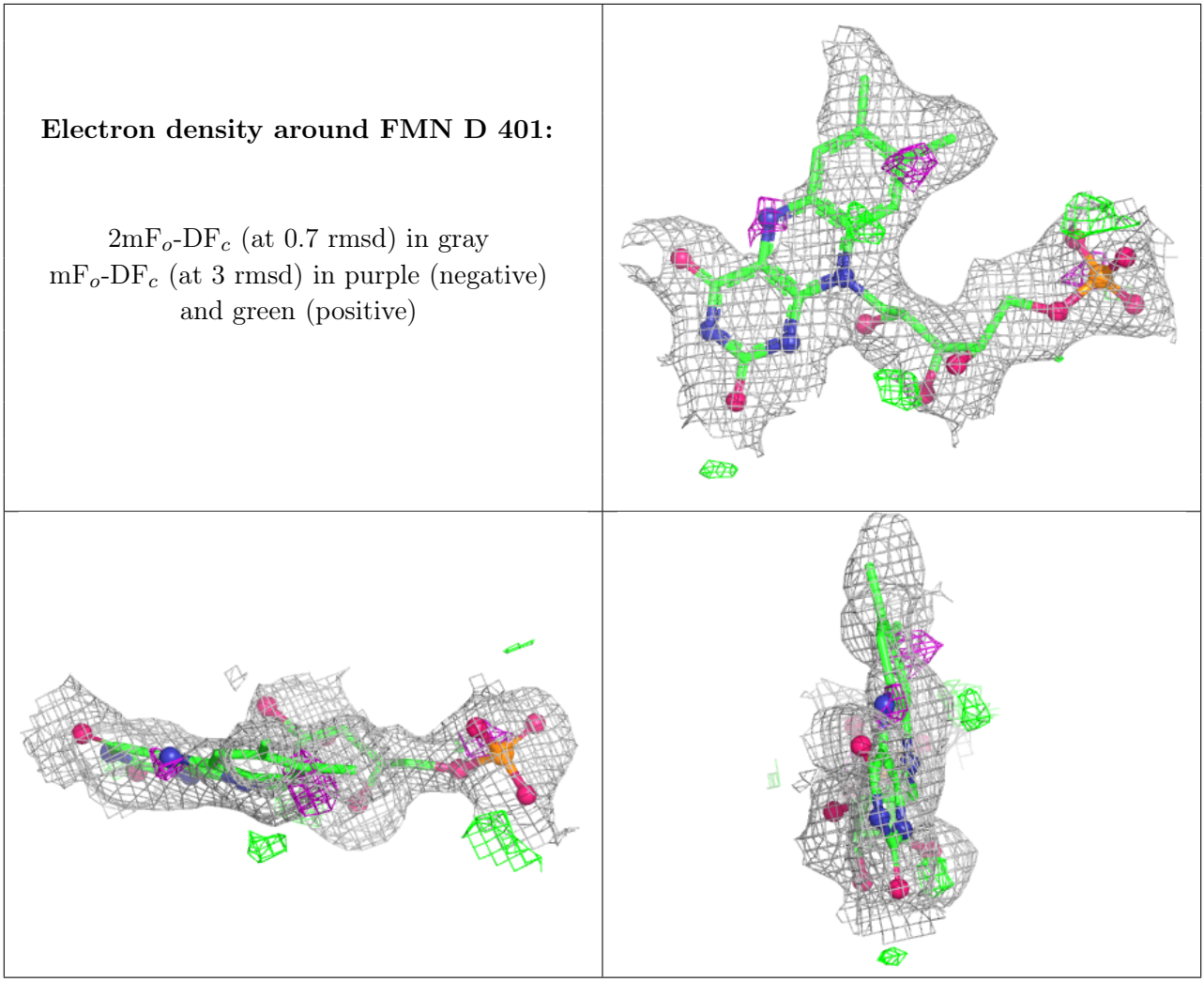






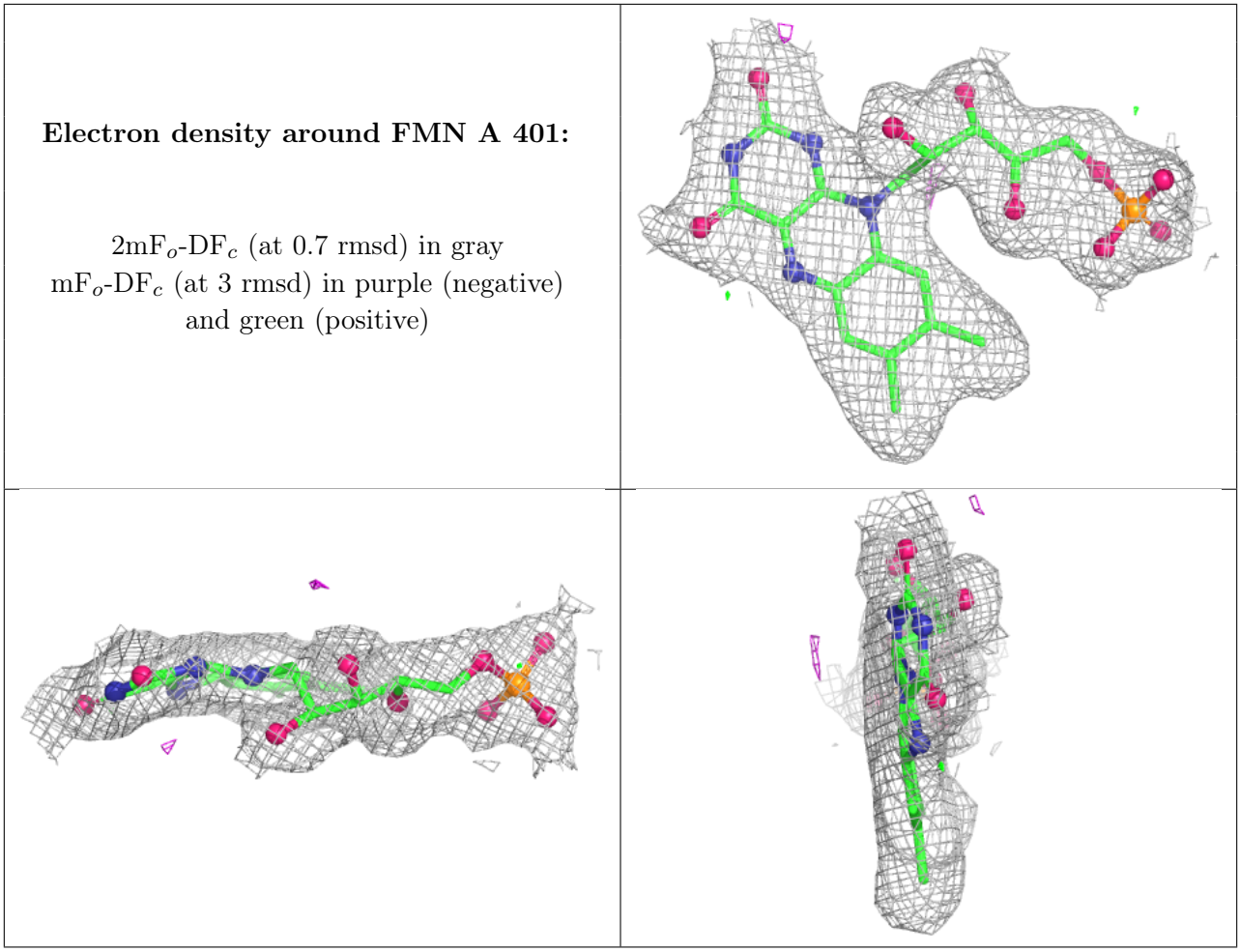
Electron density around FMN D 401:

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



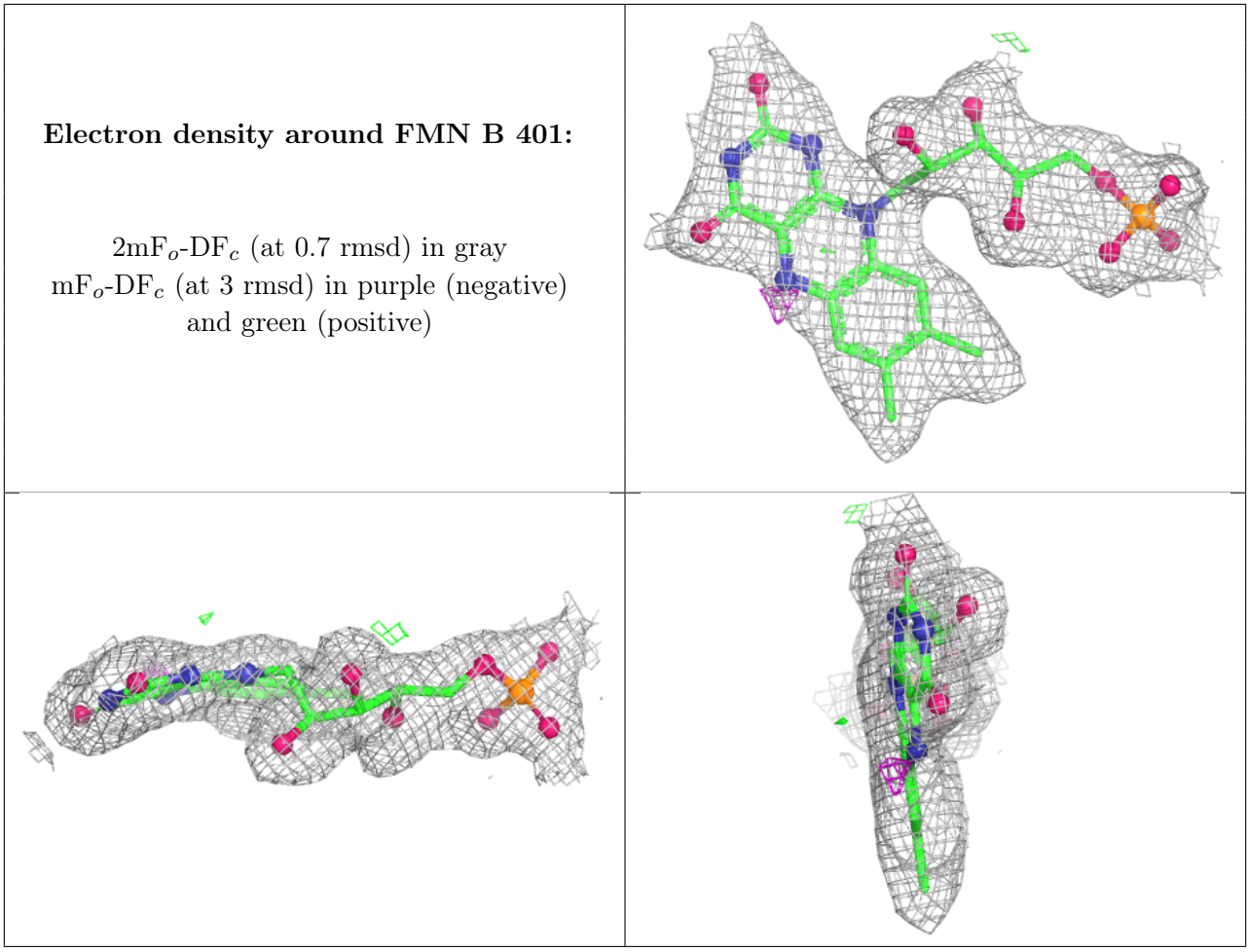
Electron density around FMN A 401:

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



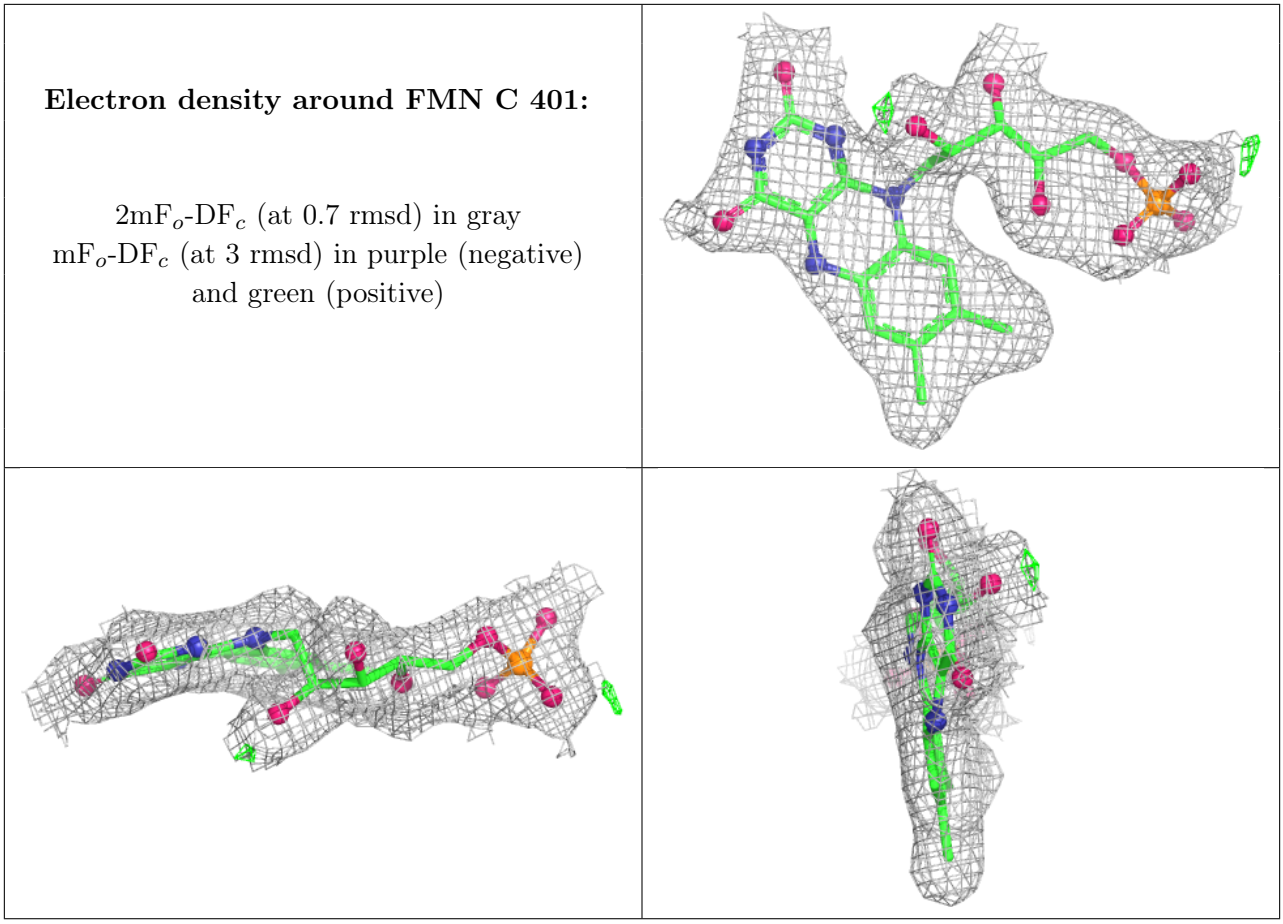
Electron density around FMN B 401:

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



Electron density around FMN C 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.