Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 07:39 AM EDT

PDB ID	:	6DVH
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 (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:

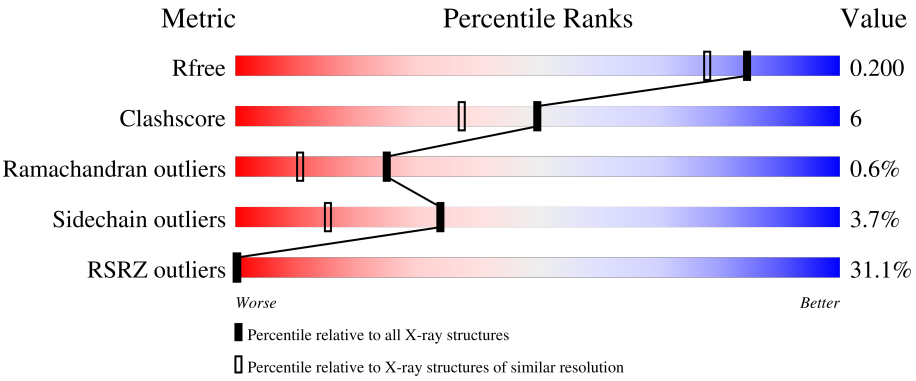
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 <=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	5% 91% 8% ·
1	B	394	13% 89% 9% ··
1	C	394	12% 92% 6% ·
1	D	394	22% 86% 13% ·
1	E	394	62% 85% 13% ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	394	

2 Entry composition (i)

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.

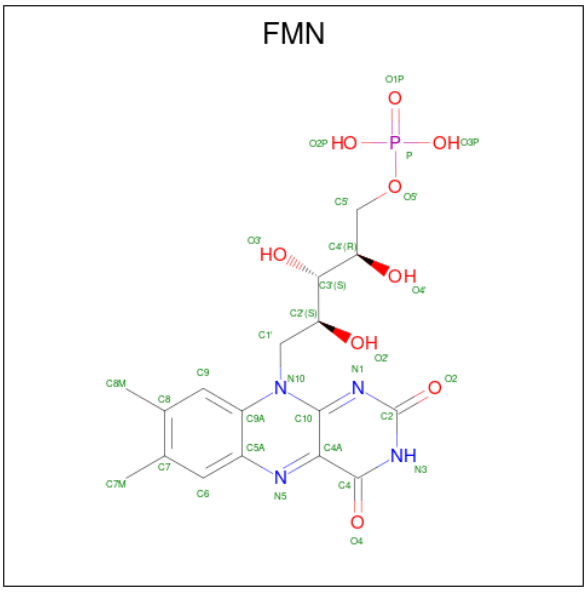
- Molecule 1 is a protein called Lactate 2-monooxygenase.

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:

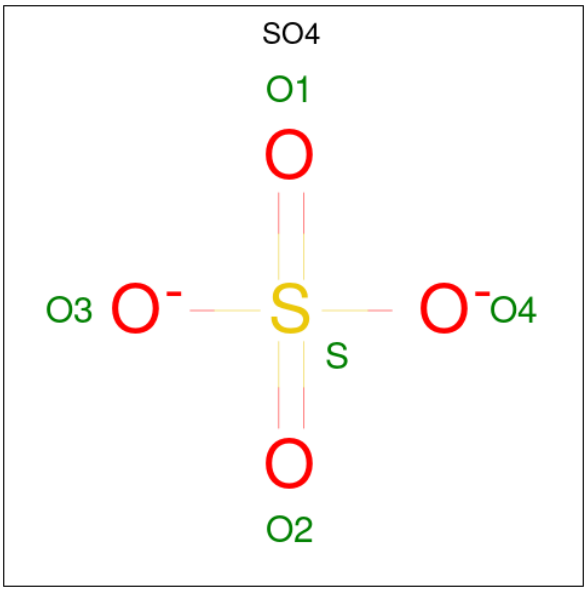
Chain	Residue	Modelled	Actual	Comment	Reference
A	203	ALA	CYS	engineered mutation	UNP P21795
B	203	ALA	CYS	engineered mutation	UNP P21795
C	203	ALA	CYS	engineered mutation	UNP P21795
D	203	ALA	CYS	engineered mutation	UNP P21795
E	203	ALA	CYS	engineered mutation	UNP P21795
F	203	ALA	CYS	engineered mutation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

- Molecule 2 is FLAVIN MONONUCLEOTIDE (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 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	1
3	A	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	B	1	Total O S 5 4 1	0	1
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	1
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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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.

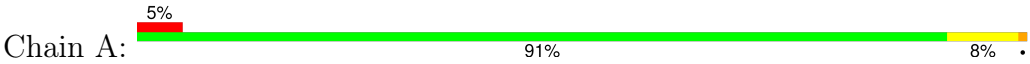
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	499	Total O 499 499	0	4
4	B	358	Total O 358 358	0	4
4	C	313	Total O 313 313	0	2
4	D	182	Total O 182 182	0	2
4	E	13	Total O 13 13	0	0
4	F	9	Total O 9 9	0	0

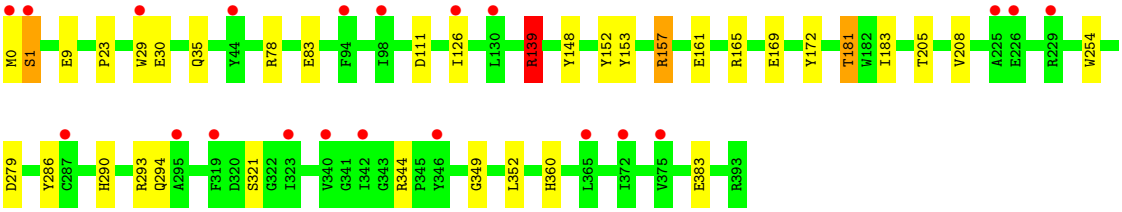
3 Residue-property plots (i)

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

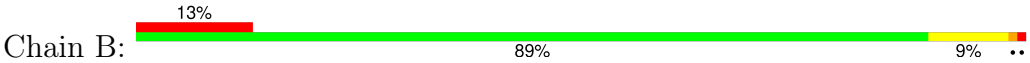
Chain A:

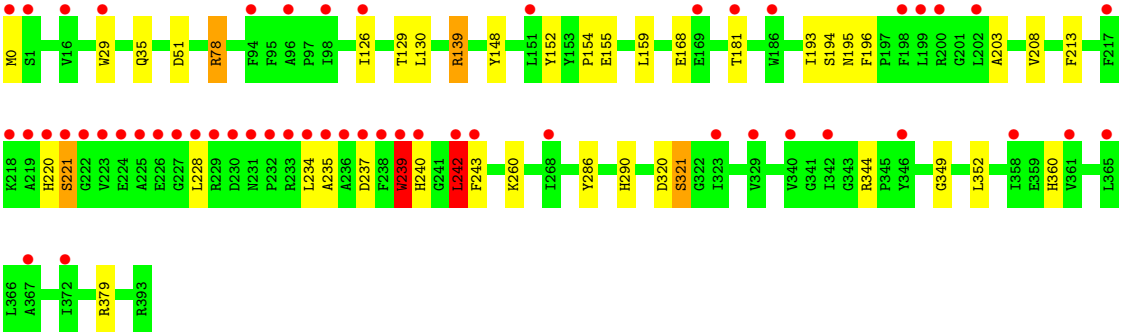




• Molecule 1: Lactate 2-monooxygenase

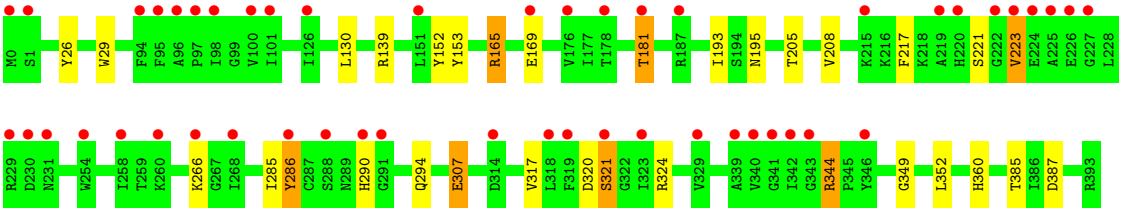
Chain B:





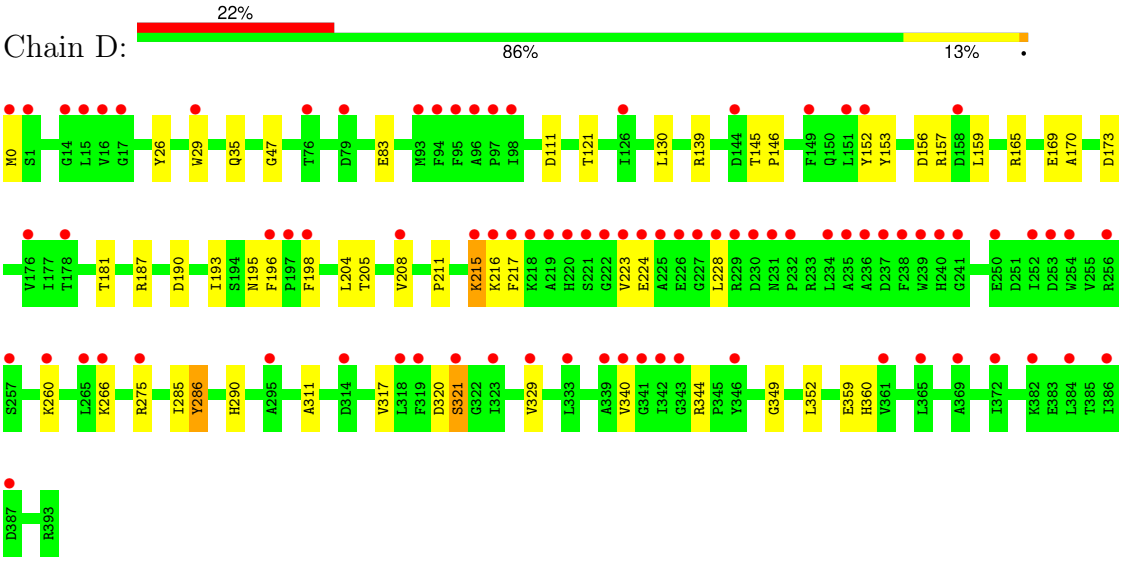
• Molecule 1: Lactate 2-monooxygenase

Chain C:



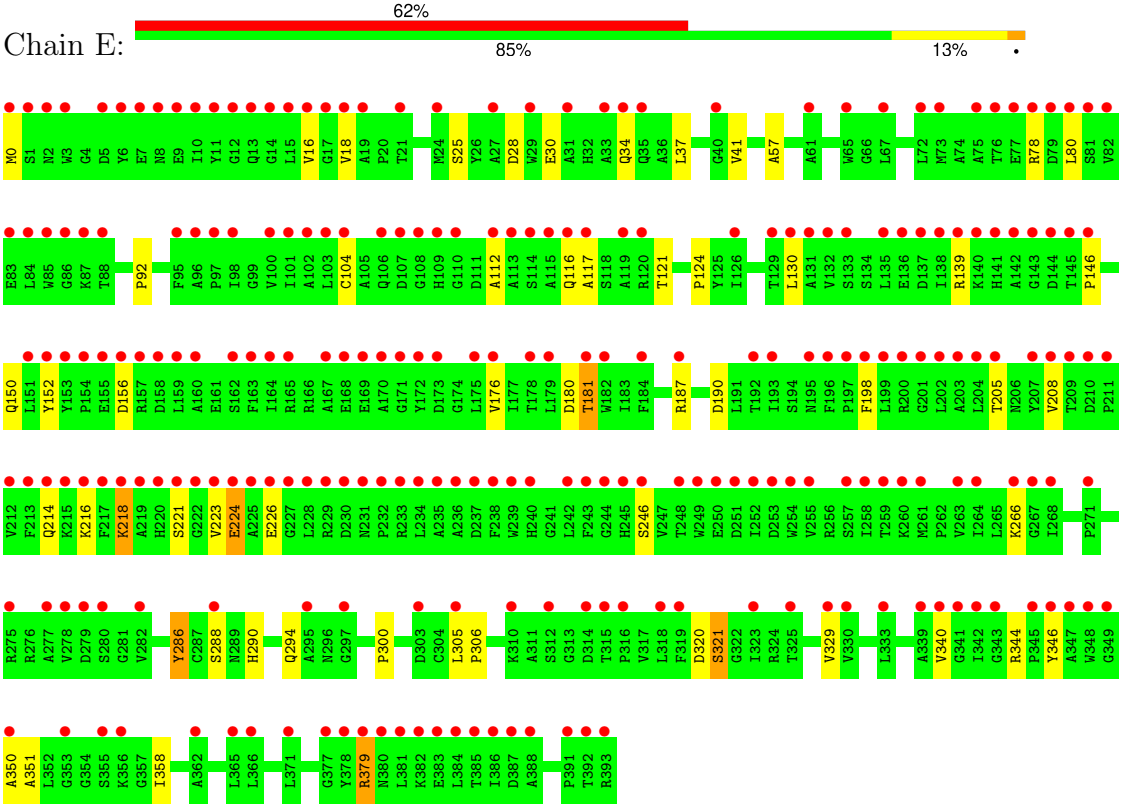
• Molecule 1: Lactate 2-monooxygenase

Chain D:



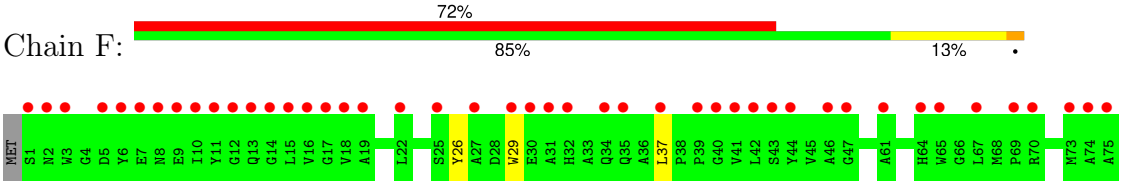
• Molecule 1: Lactate 2-monooxygenase

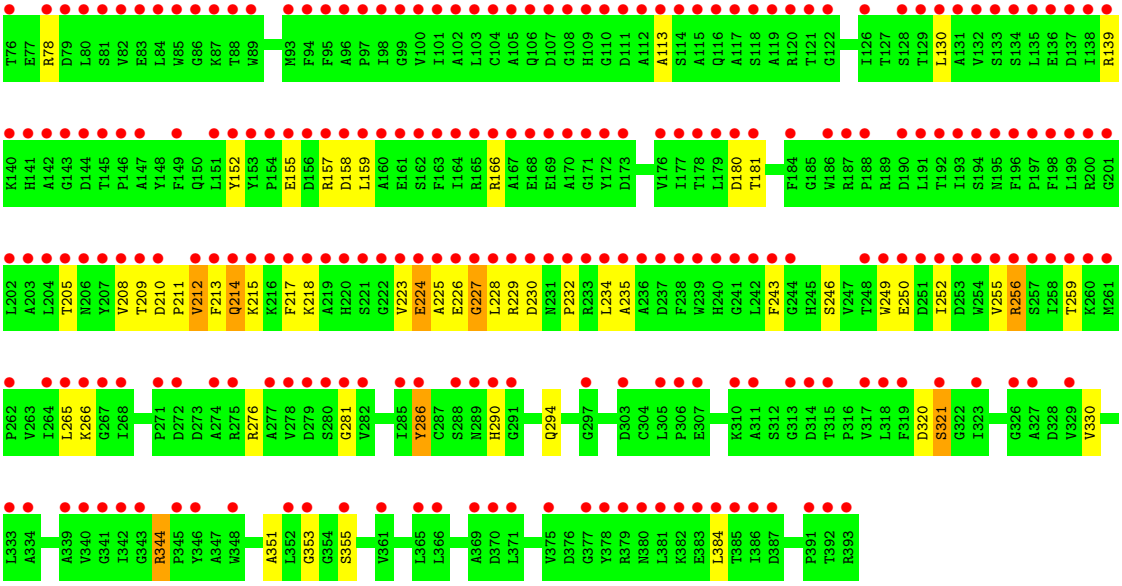
Chain E:



• Molecule 1: Lactate 2-monooxygenase

Chain F:




T76 E77 R78 D79 L80 S81 V82 E83 L84 W85 G86 K87 T88 W89
M93 F94 F95 A96 P97 I98 G99 V100 I101 A102 L103 C104 A105 Q106 D107 G108 H109 G110 D111 A112 A113 S114 A115 Q116 A117 S118 A119 R120 T121 G122
I126 T127 S128 T129 L130 A131 V132 S133 S134 L135 E136 D137 I138 R139
K140 H141 A142 G143 D144 T145 P146 A147 Y148 F149 Q150 L151 Y152 Y153 P154 E155 D156 R157 D158 L159 A160 E161 S162 F163 I164 R165 R166 A167 E168 E169 A170 G171 Y172 D173
V176 I177 T178 L179 D180 T181
F184 G185 W186 R187 P188 R189 D190 L191 T192 I193 S194 N195 F196 P197 F198 L199 R200 G201
L202 A203 L204 T205 N206 Y207 V208 T209 D210 P211 V212 F213 Q214 K215 K216 F217 K218 A219 H220 S221 G222 V223 E224 A225 E226 G227 L228 R229 D230 W231 P232 R233 L234 A235 A236 D237 F238 W239 H240 G241 L242 F243 G244 H245 S246 V247 T248 W249 E250 D251 I252 D253 W254 V255 R256 S257 I258 T259 K260 M261
P262 V263 I264 L265 K266 G267 I268 P271 D272 D273 A274 R275 R276 A277 V278 D279 S280 G281 V282 I285 Y286 C287 S288 N289 H290 G291 Q294 G297 D303 C304 L305 P306 E307 K310 A311 S312 G313 D314 T315 P316 V317 L318 F319 D320 S321 G322 I323 G326 A327 D328 V329 V330
L333 A334 A339 V340 G341 I342 G343 R344 P345 Y346 A347 W348 A351 L352 G353 G354 S355 Y361 L365 L366 A369 D370 L371 V375 D376 G377 Y378 R379 N380 L381 K382 E383 L384 T385 I386 D387 P391 T392 R393

4 Data and refinement statistics (i)

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) 100.0 (30.90-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (10.06%)	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)	0.32 , 58.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[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: FMN, SO4

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	1/3197 (0.0%)	0.86	3/4353 (0.1%)
1	B	0.70	1/3286 (0.0%)	0.80	6/4473 (0.1%)
1	C	0.63	0/3168	0.71	1/4311 (0.0%)
1	D	0.51	0/3164	0.60	0/4306
1	E	0.36	0/3140	0.49	0/4275
1	F	0.34	0/3134	0.51	0/4268
All	All	0.60	2/19089 (0.0%)	0.68	10/25986 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	GLU	CD-OE2	-8.02	1.16	1.25
1	B	78	ARG	CG-CD	-5.07	1.39	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	78	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	B	78	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	139	ARG	NE-CZ-NH1	-6.09	117.25	120.30
1	A	111	ASP	CB-CG-OD1	6.04	123.74	118.30
1	B	78	ARG	CA-CB-CG	-5.82	100.59	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	344	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	B	51	ASP	CB-CG-OD1	5.22	123.00	118.30
1	B	242[A]	LEU	CB-CG-CD2	5.20	119.84	111.00
1	B	242[B]	LEU	CB-CG-CD2	5.20	119.84	111.00
1	A	293	ARG	NE-CZ-NH1	-5.08	117.76	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	239[A]	TRP	Peptide
1	B	242[A]	LEU	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	3080	0	3026	24	0
1	B	3166	0	3083	44	0
1	C	3066	0	3002	28	0
1	D	3062	0	2997	38	0
1	E	3043	0	2978	33	0
1	F	3037	0	2975	45	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	0	0
2	F	31	0	19	1	0
3	A	20	0	0	0	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	6	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	213	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 (213) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD1	1:B:237[B]:ASP:N	2.33	0.62
1:B:29[B]:TRP:CZ3	1:B:352:LEU:HD12	2.37	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
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: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: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:HA	1:B:239[A]:TRP:CE3	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:211:PRO:O	1:F:214:GLN:C	2.48	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:F:226:GLU:C	1:F:228:LEU:N	2.64	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: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:B:242[A]:LEU:HD12	1:B:242[A]:LEU:C	2.32	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:288:SER:OG	1:E:320:ASP:OD1	2.27	0.48
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:193:ILE:O	1:B:194:SER:C	2.51	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
1:C:181[B]:THR:CG2	1:C:290:HIS:CE1	2.98	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: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:A:139:ARG:HG2	1:A:172:TYR:CE2	2.51	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: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:D:329:VAL:HG13	1:D:340[B]:VAL:CG2	2.39	0.45
1:E:320:ASP:OD1	1:E:320:ASP:C	2.56	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:104:CYS:O	1:E:351:ALA:HA	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:117:ALA:O	1:E:121:THR:HG23	2.18	0.43
1:A:205:THR:HA	1:A:208[A]:VAL:CG2	2.48	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: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:C:385:THR:OG1	1:C:387:ASP:OD1	2.27	0.42
1:E:156:ASP:OD2	1:E:216:LYS:HE3	2.18	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
2:D:401:FMN:H9	2:D:401:FMN:O4'	2.20	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:B:181[A]:THR:CG2	1:B:290:HIS:CE1	3.03	0.41
1:D:320:ASP:OD1	1:D:320:ASP:C	2.59	0.41
1:E:57:ALA:HB1	1:E:300:PRO:HG3	2.03	0.41
1:B:242[B]:LEU:N	1:B:242[B]:LEU:HD13	2.35	0.41
1:C:26:TYR:HA	1:C:29[A]:TRP:CE3	2.55	0.41
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181[B]:THR:HG21	1:F:290:HIS:CE1	2.55	0.41
1:D:224:GLU:H	1:D:224:GLU:CD	2.24	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:CZ	1:E:379:ARG:HB2	2.51	0.41
1:E:218:LYS:HE3	1:E:224:GLU:CD	2.42	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:C:320:ASP:OD1	1:C:320:ASP:C	2.59	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 (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	404/394 (102%)	392 (97%)	10 (2%)	2 (0%)	29 13
1	B	414/394 (105%)	397 (96%)	12 (3%)	5 (1%)	13 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	399/394 (101%)	389 (98%)	9 (2%)	1 (0%)	41 24
1	D	399/394 (101%)	388 (97%)	10 (2%)	1 (0%)	41 24
1	E	398/394 (101%)	384 (96%)	13 (3%)	1 (0%)	41 24
1	F	397/394 (101%)	373 (94%)	20 (5%)	4 (1%)	15 4
All	All	2411/2364 (102%)	2323 (96%)	74 (3%)	14 (1%)	25 11

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 (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	316/304 (104%)	304 (96%)	12 (4%)	33 14
1	B	322/304 (106%)	312 (97%)	10 (3%)	40 21
1	C	311/304 (102%)	300 (96%)	11 (4%)	36 17
1	D	311/304 (102%)	298 (96%)	13 (4%)	30 12
1	E	310/304 (102%)	296 (96%)	14 (4%)	27 10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	309/304 (102%)	296 (96%)	13 (4%)	30 12
All	All	1879/1824 (103%)	1806 (96%)	73 (4%)	34 13

All (73) 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	78	ARG
1	A	83	GLU
1	A	139	ARG
1	A	153	TYR
1	A	157	ARG
1	A	181[A]	THR
1	A	181[B]	THR
1	A	286	TYR
1	A	344	ARG
1	B	0	MET
1	B	139	ARG
1	B	159	LEU
1	B	196	PHE
1	B	208	VAL
1	B	242[A]	LEU
1	B	242[B]	LEU
1	B	260	LYS
1	B	286	TYR
1	B	344	ARG
1	C	130	LEU
1	C	139[A]	ARG
1	C	139[B]	ARG
1	C	153	TYR
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	153	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	157	ARG
1	D	159	LEU
1	D	165	ARG
1	D	169	GLU
1	D	196	PHE
1	D	204	LEU
1	D	215	LYS
1	D	260	LYS
1	D	286	TYR
1	D	344	ARG
1	E	0	MET
1	E	78	ARG
1	E	139	ARG
1	E	152	TYR
1	E	181[A]	THR
1	E	181[B]	THR
1	E	218	LYS
1	E	224	GLU
1	E	226	GLU
1	E	246	SER
1	E	286	TYR
1	E	344	ARG
1	E	346	TYR
1	E	379	ARG
1	F	78	ARG
1	F	139	ARG
1	F	152	TYR
1	F	155	GLU
1	F	157	ARG
1	F	158	ASP
1	F	212	VAL
1	F	214	GLN
1	F	229	ARG
1	F	246	SER
1	F	256	ARG
1	F	286	TYR
1	F	344	ARG

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	D	403	-	4,4,4	0.49	0	6,6,6	0.39	0
3	SO4	D	402	-	4,4,4	0.38	0	6,6,6	0.70	0
3	SO4	B	402	-	4,4,4	0.62	0	6,6,6	0.46	0
3	SO4	B	404[A]	-	4,4,4	0.31	0	6,6,6	0.11	0
3	SO4	B	403	-	4,4,4	0.26	0	6,6,6	0.37	0
3	SO4	A	404[A]	-	4,4,4	0.36	0	6,6,6	0.61	0
3	SO4	A	405	-	4,4,4	0.36	0	6,6,6	0.17	0
3	SO4	E	403	-	4,4,4	0.24	0	6,6,6	0.23	0
3	SO4	C	402	-	4,4,4	0.36	0	6,6,6	0.72	0
2	FMN	C	401	-	33,33,33	1.86	7 (21%)	48,50,50	1.25	6 (12%)
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	B	406[B]	-	4,4,4	0.48	0	6,6,6	0.36	0
3	SO4	F	403	-	4,4,4	0.28	0	6,6,6	0.27	0
3	SO4	A	403	-	4,4,4	0.47	0	6,6,6	0.62	0
3	SO4	A	402	-	4,4,4	0.53	0	6,6,6	0.80	0
2	FMN	E	401	-	33,33,33	1.59	5 (15%)	48,50,50	1.36	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SO4	F	402	-	4,4,4	0.23	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	C	404	-	4,4,4	0.28	0	6,6,6	0.20	0
2	FMN	B	401	-	33,33,33	1.93	7 (21%)	48,50,50	1.46	9 (18%)
2	FMN	F	401	-	33,33,33	1.57	4 (12%)	48,50,50	1.33	7 (14%)
3	SO4	B	405	-	4,4,4	0.20	0	6,6,6	0.14	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	E	401	-	-	5/18/18/18	0/3/3/3
2	FMN	F	401	-	-	5/18/18/18	0/3/3/3
2	FMN	C	401	-	-	1/18/18/18	0/3/3/3
2	FMN	D	401	-	-	1/18/18/18	0/3/3/3
2	FMN	B	401	-	-	1/18/18/18	0/3/3/3
2	FMN	A	401	-	-	1/18/18/18	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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(^{o})	Ideal(^{o})
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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'

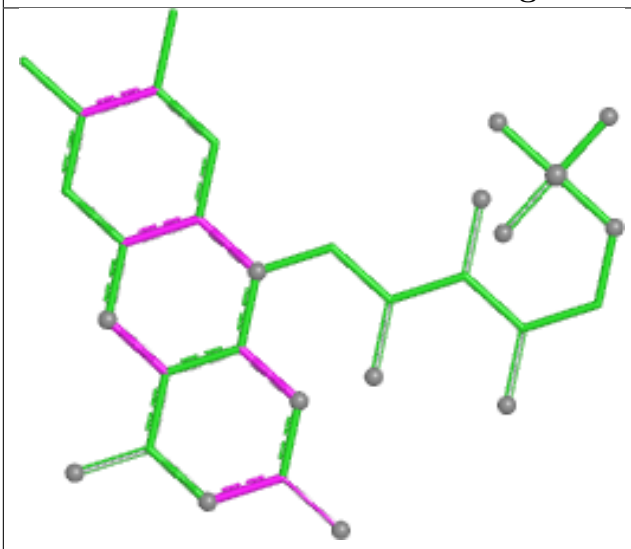
There are no ring outliers.

3 monomers are involved in 3 short contacts:

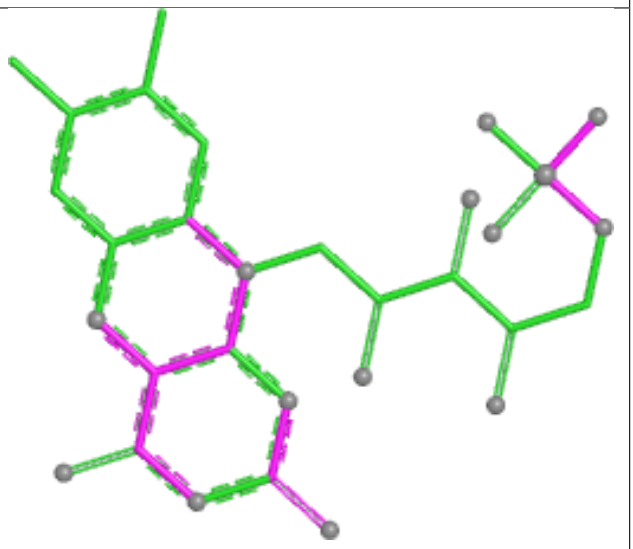
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	FMN	1	0
2	D	401	FMN	1	0
2	F	401	FMN	1	0

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 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.

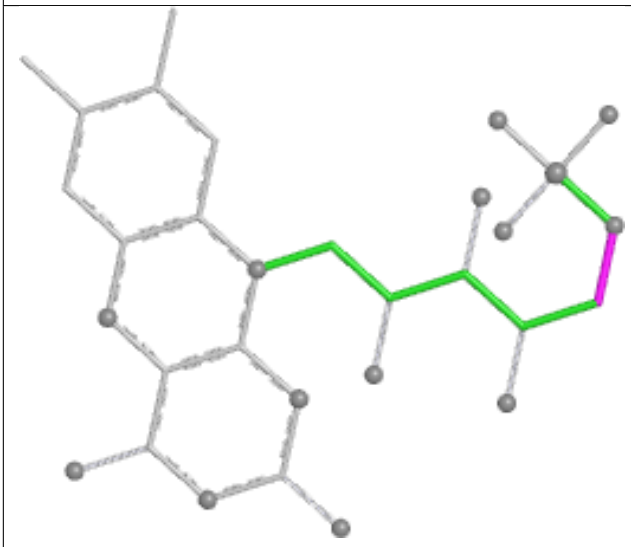
Ligand FMN C 401



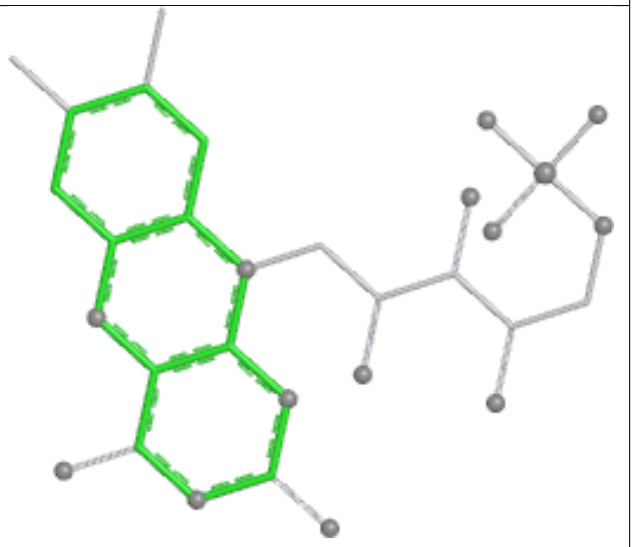
Bond lengths



Bond angles

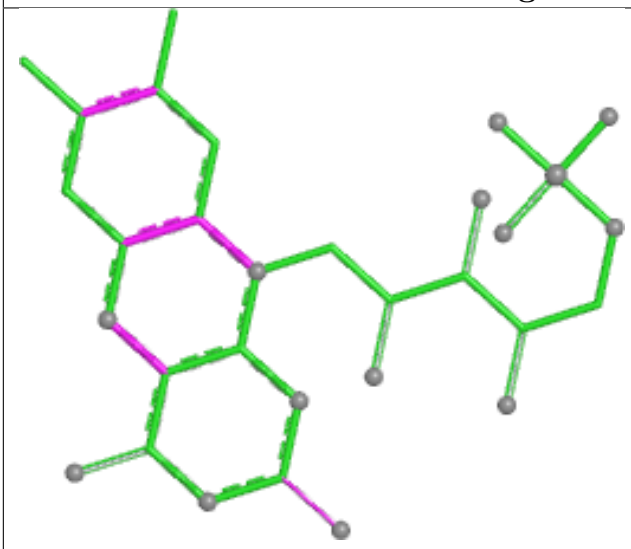


Torsions

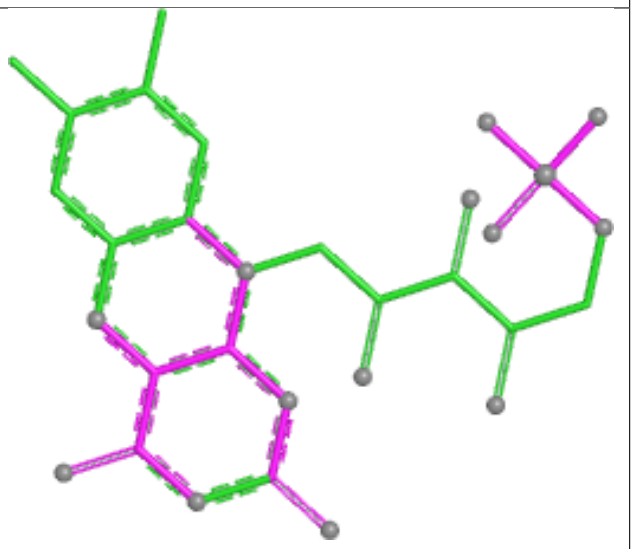


Rings

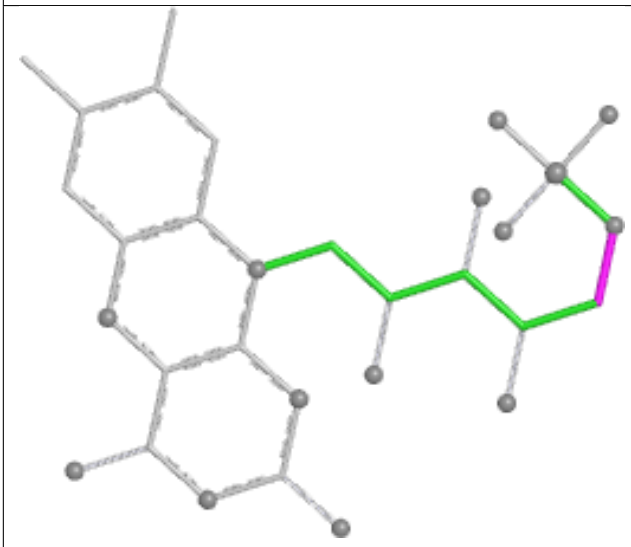
Ligand FMN D 401



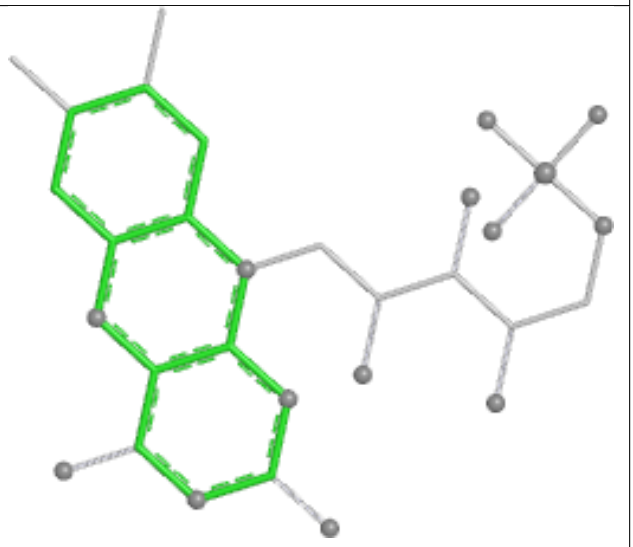
Bond lengths



Bond angles

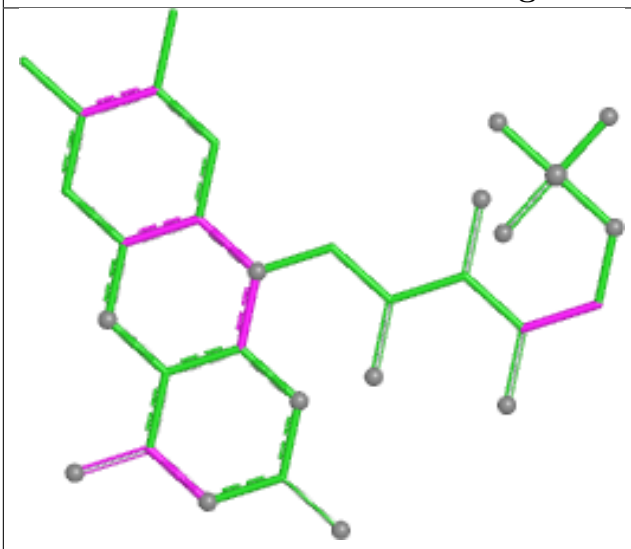


Torsions

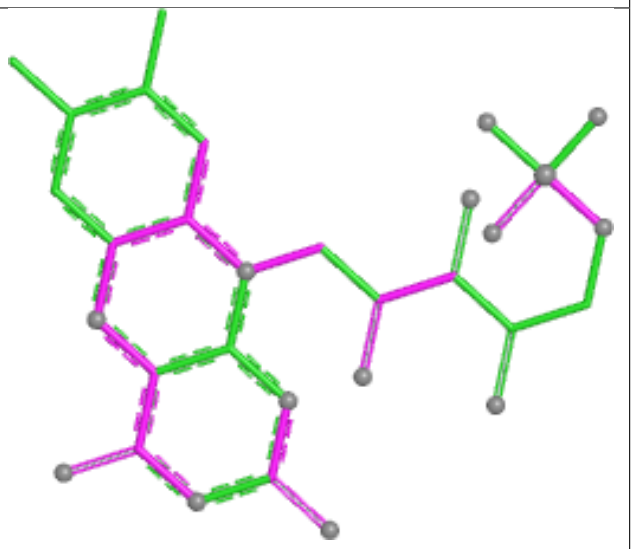


Rings

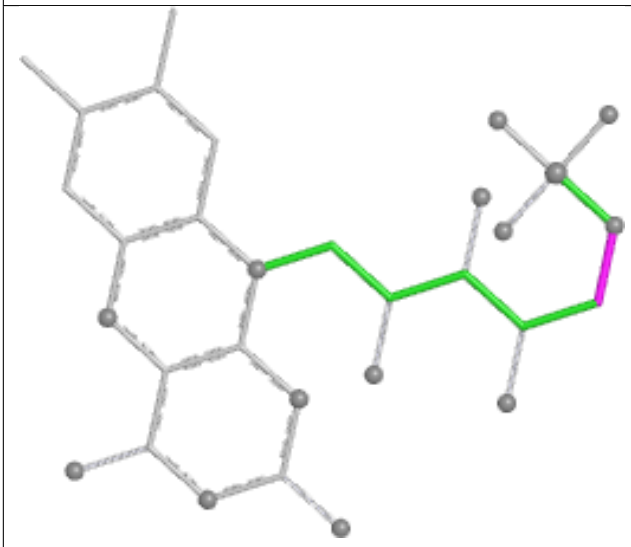
Ligand FMN A 401



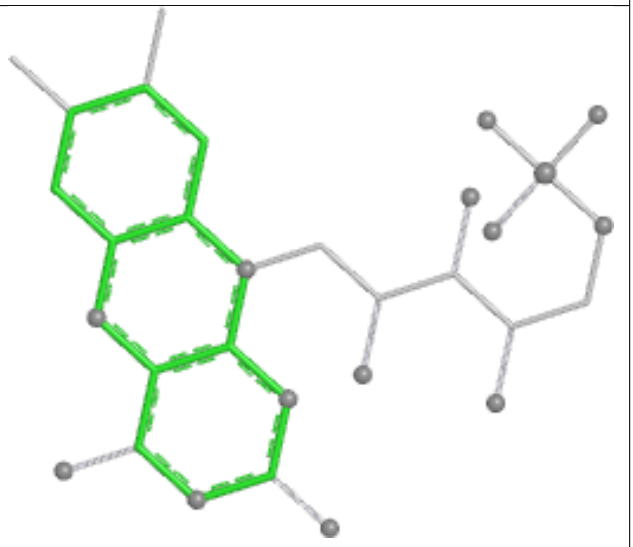
Bond lengths



Bond angles

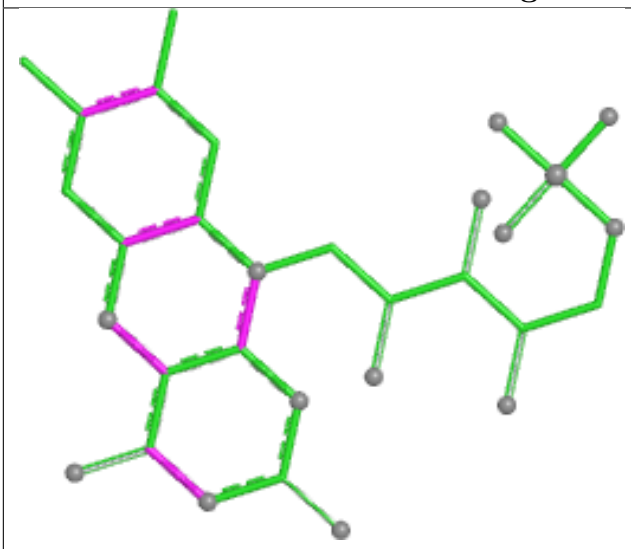


Torsions

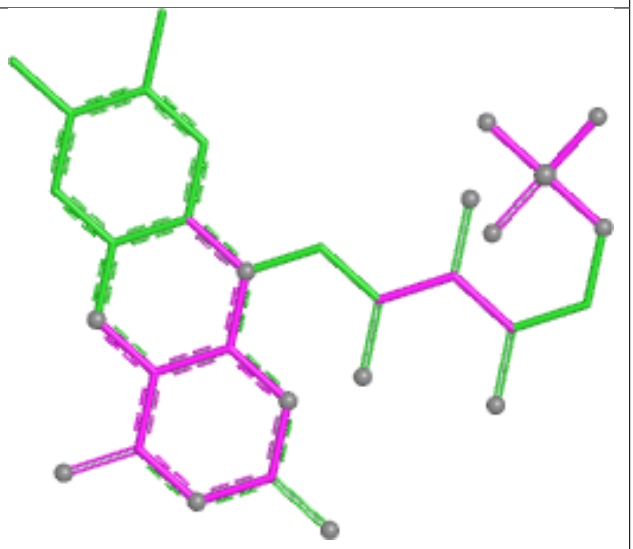


Rings

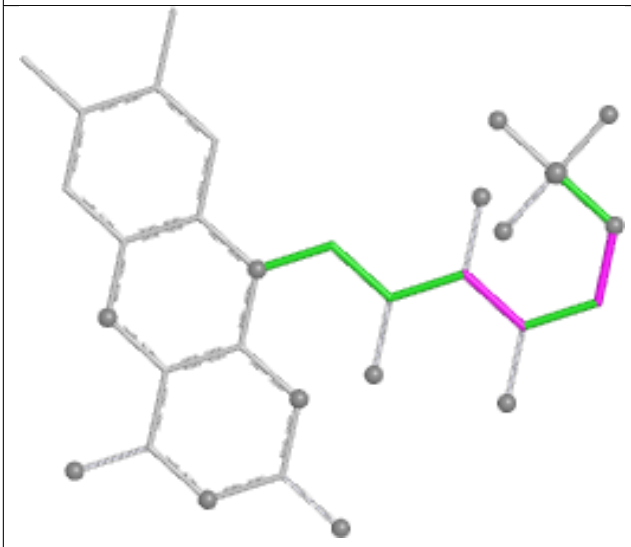
Ligand FMN E 401



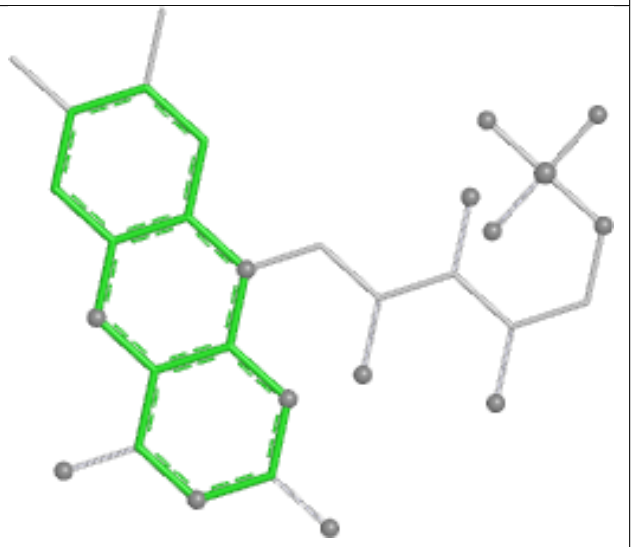
Bond lengths



Bond angles

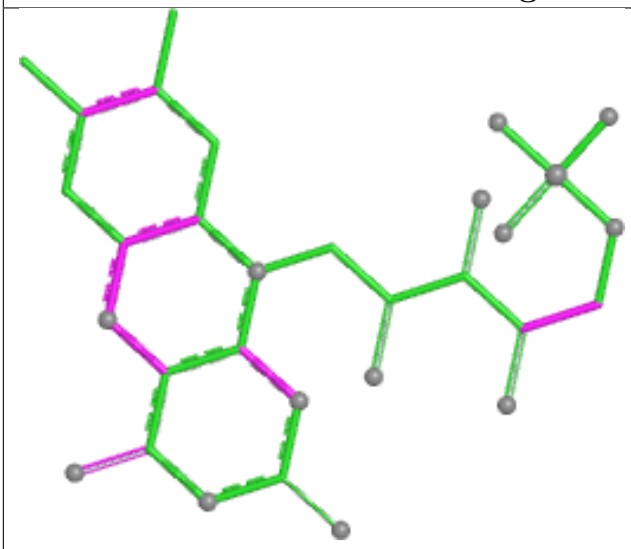


Torsions

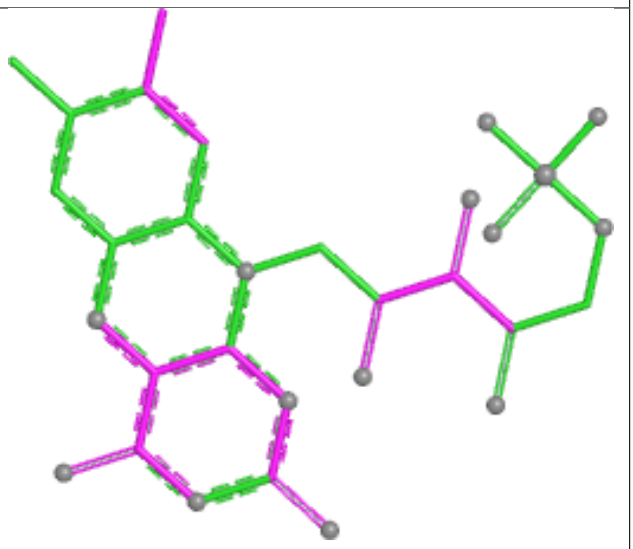


Rings

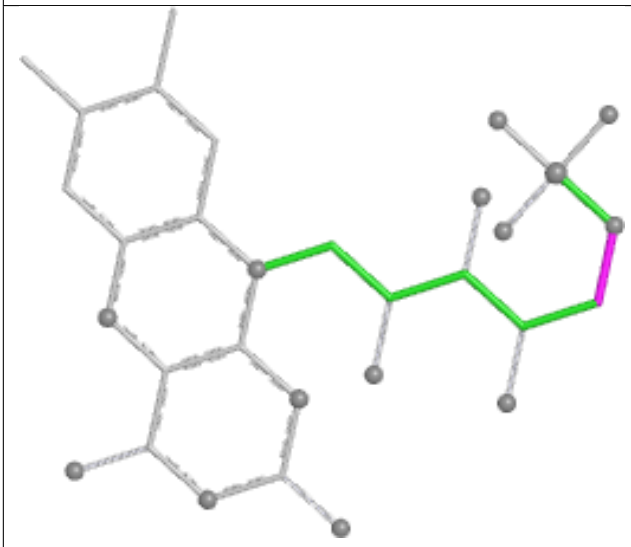
Ligand FMN B 401



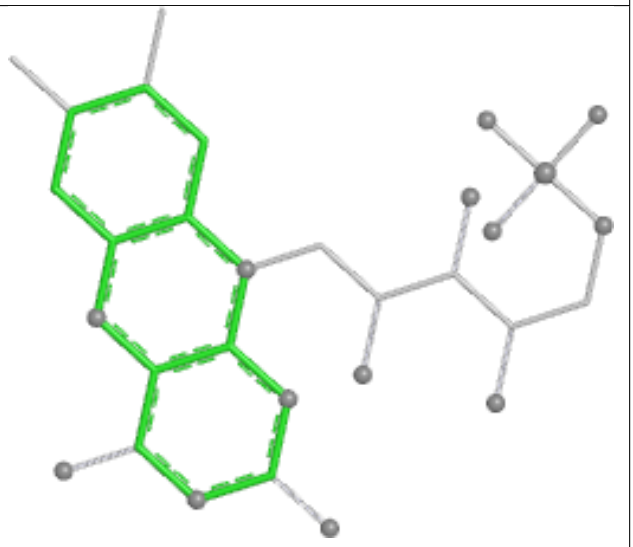
Bond lengths



Bond angles

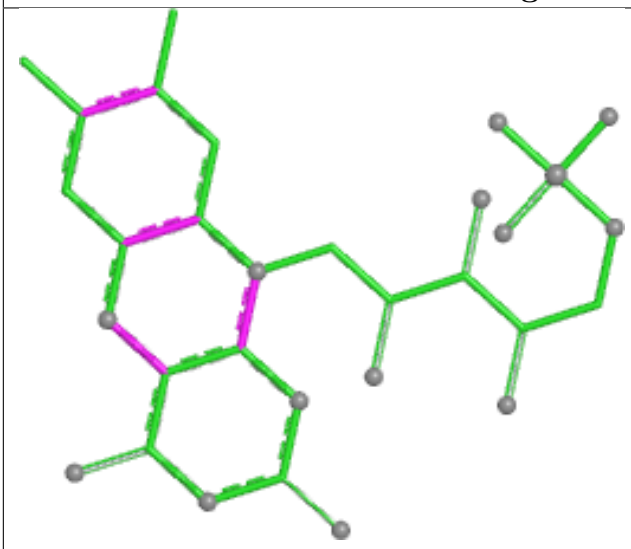


Torsions

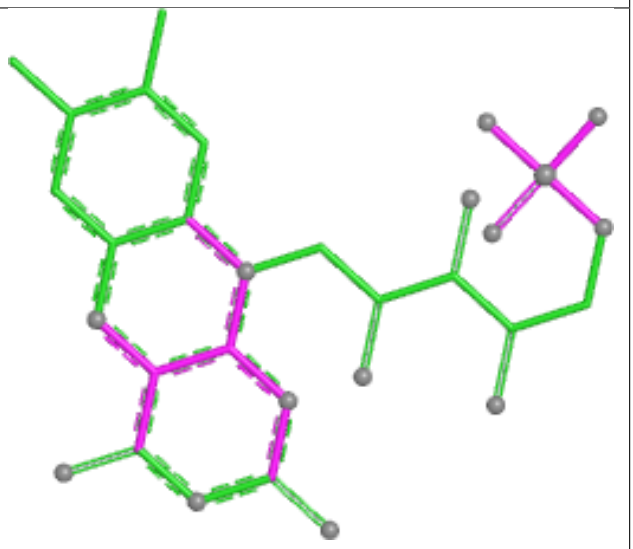


Rings

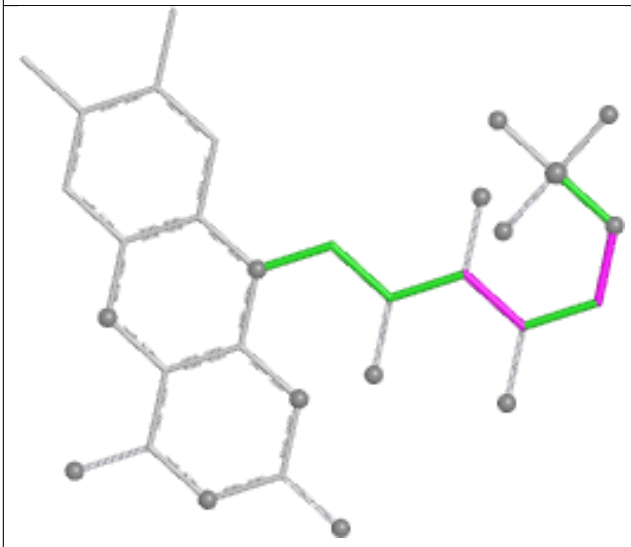
Ligand FMN F 401



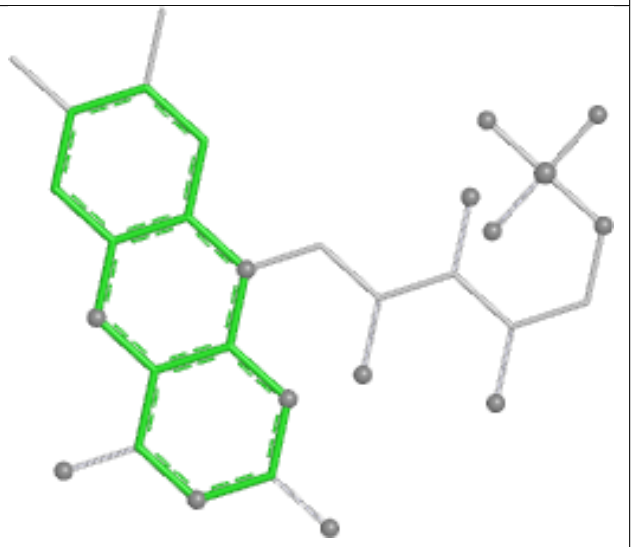
Bond lengths



Bond angles



Torsions



Rings

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%)	0.30	21 (5%) 26 29	19, 30, 49, 77	0
1	B	394/394 (100%)	0.67	53 (13%) 3 3	25, 38, 88, 131	0
1	C	394/394 (100%)	0.48	49 (12%) 4 4	30, 43, 70, 100	0
1	D	394/394 (100%)	1.17	85 (21%) 0 0	46, 62, 103, 160	0
1	E	394/394 (100%)	3.44	243 (61%) 0 0	72, 103, 158, 190	394 (100%)
1	F	393/394 (99%)	4.08	285 (72%) 0 0	87, 113, 169, 204	393 (100%)
All	All	2363/2364 (99%)	1.69	736 (31%) 0 0	19, 57, 137, 204	787 (33%)

All (736) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	223	VAL	28.0
1	E	238	PHE	23.7
1	E	234	LEU	22.1
1	F	222	GLY	19.7
1	F	226	GLU	19.0
1	E	236	ALA	18.9
1	F	239	TRP	17.4
1	E	239	TRP	17.0
1	F	228	LEU	16.8
1	E	235	ALA	15.7
1	E	229	ARG	15.6
1	F	213	PHE	15.2
1	F	230	ASP	14.8
1	F	236	ALA	14.7
1	F	235	ALA	14.5
1	E	223	VAL	13.4
1	F	234	LEU	13.3
1	F	238	PHE	12.9
1	F	225	ALA	12.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	217	PHE	12.2
1	E	198	PHE	12.1
1	F	172	TYR	12.0
1	E	16	VAL	11.9
1	F	227	GLY	11.8
1	D	225	ALA	11.4
1	F	159	LEU	11.4
1	E	227	GLY	11.4
1	F	15	LEU	11.3
1	E	0	MET	10.9
1	E	222	GLY	10.7
1	F	219	ALA	10.7
1	F	221	SER	10.5
1	F	258	ILE	10.5
1	E	224	GLU	10.4
1	E	225	ALA	10.2
1	F	212	VAL	10.0
1	E	228	LEU	9.9
1	E	254	TRP	9.9
1	E	230	ASP	9.9
1	E	172	TYR	9.8
1	F	229	ARG	9.8
1	F	19	ALA	9.6
1	F	254	TRP	9.5
1	D	220	HIS	9.5
1	E	212	VAL	9.4
1	E	231	ASN	9.3
1	F	163	PHE	9.3
1	F	142	ALA	9.3
1	E	1	SER	9.2
1	F	220	HIS	9.1
1	F	16	VAL	9.1
1	F	199	LEU	9.0
1	E	240	HIS	8.9
1	E	219	ALA	8.9
1	F	231	ASN	8.9
1	D	239	TRP	8.8
1	E	15	LEU	8.8
1	F	18	VAL	8.8
1	E	226	GLU	8.8
1	F	217	PHE	8.7
1	E	12	GLY	8.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	259	THR	8.5
1	E	132	VAL	8.5
1	F	17	GLY	8.5
1	F	99	GLY	8.5
1	F	14	GLY	8.4
1	D	0	MET	8.3
1	F	37	LEU	8.3
1	D	226	GLU	8.3
1	E	10	ILE	8.3
1	F	88	THR	8.2
1	B	220	HIS	8.1
1	E	17	GLY	8.1
1	F	12	GLY	8.1
1	E	220	HIS	8.0
1	F	198	PHE	8.0
1	B	234	LEU	8.0
1	E	130[A]	LEU	8.0
1	B	235[A]	ALA	7.9
1	F	76	THR	7.9
1	E	18	VAL	7.9
1	E	221	SER	7.9
1	D	217	PHE	7.9
1	F	143	GLY	7.8
1	D	238	PHE	7.7
1	F	257	SER	7.7
1	E	208[A]	VAL	7.7
1	F	286	TYR	7.6
1	F	196	PHE	7.6
1	D	219	ALA	7.6
1	F	260	LYS	7.5
1	D	236	ALA	7.4
1	F	164	ILE	7.4
1	E	201	GLY	7.4
1	F	195	ASN	7.4
1	E	213	PHE	7.3
1	F	318	LEU	7.2
1	F	65	TRP	7.2
1	F	266	LYS	7.2
1	F	97	PRO	7.1
1	F	208[A]	VAL	7.1
1	E	14	GLY	7.0
1	F	170	ALA	7.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	210	ASP	7.0
1	B	0	MET	7.0
1	F	140	LYS	7.0
1	E	165	ARG	7.0
1	E	193	ILE	6.9
1	D	221	SER	6.9
1	D	234	LEU	6.9
1	E	199	LEU	6.9
1	F	138	ILE	6.8
1	F	265	LEU	6.8
1	F	207	TYR	6.8
1	F	79	ASP	6.8
1	E	131	ALA	6.7
1	E	237	ASP	6.7
1	D	227	GLY	6.7
1	D	230	ASP	6.7
1	B	230	ASP	6.6
1	F	342	ILE	6.6
1	E	377	GLY	6.6
1	E	101	ILE	6.6
1	B	221	SER	6.6
1	F	8	ASN	6.6
1	E	260	LYS	6.6
1	F	85	TRP	6.5
1	F	386	ILE	6.5
1	A	0	MET	6.5
1	D	340[A]	VAL	6.5
1	F	144	ASP	6.5
1	F	261	MET	6.5
1	E	255	VAL	6.5
1	B	239[A]	TRP	6.5
1	E	98	ILE	6.4
1	F	11	TYR	6.4
1	F	98	ILE	6.4
1	E	135	LEU	6.4
1	E	209	THR	6.4
1	E	144	ASP	6.4
1	F	224	GLU	6.3
1	F	42	LEU	6.3
1	E	232	PRO	6.3
1	F	131	ALA	6.3
1	F	218	LYS	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	250	GLU	6.3
1	B	227	GLY	6.3
1	F	70	ARG	6.3
1	B	225	ALA	6.3
1	D	235	ALA	6.3
1	F	365	LEU	6.2
1	E	83	GLU	6.2
1	F	75	ALA	6.2
1	E	382	LYS	6.2
1	D	224	GLU	6.2
1	F	253	ASP	6.2
1	B	238[A]	PHE	6.2
1	F	169	GLU	6.2
1	F	10	ILE	6.1
1	F	101	ILE	6.1
1	F	153	TYR	6.1
1	F	135	LEU	6.1
1	F	381	LEU	6.1
1	F	156	ASP	6.1
1	F	244	GLY	6.1
1	F	152	TYR	6.1
1	E	145	THR	6.1
1	F	41	VAL	6.1
1	F	237	ASP	6.0
1	F	197	PRO	6.0
1	F	250	GLU	6.0
1	F	340[A]	VAL	6.0
1	B	228	LEU	6.0
1	E	138	ILE	6.0
1	F	86	GLY	5.9
1	E	323	ILE	5.9
1	F	178	THR	5.9
1	F	200	ARG	5.8
1	F	233	ARG	5.8
1	E	86	GLY	5.8
1	D	228	LEU	5.8
1	F	40	GLY	5.8
1	F	341	GLY	5.8
1	F	385	THR	5.8
1	B	223	VAL	5.7
1	F	380	ASN	5.7
1	B	243[A]	PHE	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	236[A]	ALA	5.7
1	E	340[A]	VAL	5.7
1	D	342	ILE	5.7
1	E	257	SER	5.6
1	F	112	ALA	5.6
1	F	343	GLY	5.6
1	B	217	PHE	5.6
1	F	305	LEU	5.6
1	E	233	ARG	5.6
1	F	393	ARG	5.6
1	C	0	MET	5.5
1	F	78	ARG	5.5
1	F	215	LYS	5.5
1	F	141	HIS	5.5
1	E	142	ALA	5.5
1	F	82	VAL	5.5
1	E	13	GLN	5.4
1	E	196	PHE	5.4
1	B	222	GLY	5.4
1	E	353	GLY	5.4
1	E	211	PRO	5.4
1	E	143	GLY	5.3
1	F	94	PHE	5.3
1	E	140	LYS	5.3
1	F	203	ALA	5.3
1	D	94	PHE	5.3
1	F	184	PHE	5.3
1	F	202	LEU	5.3
1	E	141	HIS	5.3
1	F	130[A]	LEU	5.3
1	E	216	LYS	5.3
1	E	342	ILE	5.3
1	F	243	PHE	5.3
1	F	122	GLY	5.2
1	E	88	THR	5.2
1	B	229	ARG	5.2
1	E	85	TRP	5.2
1	E	151	LEU	5.2
1	E	76	THR	5.2
1	F	242	LEU	5.2
1	E	169	GLU	5.1
1	E	381	LEU	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	11	TYR	5.1
1	F	181[A]	THR	5.1
1	E	379	ARG	5.1
1	E	258	ILE	5.0
1	E	386	ILE	5.0
1	C	226	GLU	5.0
1	F	366	LEU	5.0
1	B	237[A]	ASP	5.0
1	F	1	SER	5.0
1	B	226	GLU	5.0
1	F	102	ALA	5.0
1	F	256	ARG	5.0
1	F	87	LYS	5.0
1	D	176	VAL	5.0
1	F	391	PRO	5.0
1	F	187[A]	ARG	5.0
1	E	242	LEU	4.9
1	E	82	VAL	4.9
1	F	176	VAL	4.9
1	D	229	ARG	4.9
1	F	382	LYS	4.9
1	E	348	TRP	4.9
1	E	253	ASP	4.9
1	F	104	CYS	4.9
1	E	195	ASN	4.9
1	D	237	ASP	4.8
1	E	9	GLU	4.8
1	F	74	ALA	4.8
1	E	176	VAL	4.8
1	F	9	GLU	4.8
1	D	223	VAL	4.8
1	E	109	HIS	4.8
1	D	222	GLY	4.8
1	F	232	PRO	4.7
1	F	7	GLU	4.7
1	F	84	LEU	4.7
1	E	152	TYR	4.7
1	E	329	VAL	4.7
1	F	378	TYR	4.7
1	F	210	ASP	4.7
1	E	384	LEU	4.7
1	F	105	ALA	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	231	ASN	4.7
1	E	218	LYS	4.6
1	D	16	VAL	4.6
1	E	346	TYR	4.6
1	C	98	ILE	4.6
1	B	231	ASN	4.6
1	F	168	GLU	4.6
1	E	385	THR	4.6
1	B	98	ILE	4.6
1	F	165	ARG	4.6
1	C	229	ARG	4.5
1	F	107	ASP	4.5
1	F	329	VAL	4.5
1	E	261	MET	4.5
1	E	207	TYR	4.5
1	C	225	ALA	4.5
1	E	110	GLY	4.5
1	F	379	ARG	4.5
1	E	266	LYS	4.5
1	E	343	GLY	4.5
1	C	126	ILE	4.5
1	D	126	ILE	4.5
1	E	116	GLN	4.5
1	F	119	ALA	4.5
1	F	193	ILE	4.4
1	F	13	GLN	4.4
1	D	365	LEU	4.4
1	E	215	LYS	4.4
1	B	219	ALA	4.4
1	E	168	GLU	4.4
1	F	137	ASP	4.4
1	E	259	THR	4.4
1	E	200	ARG	4.3
1	D	29[A]	TRP	4.3
1	F	96	ALA	4.3
1	F	319	PHE	4.3
1	F	157	ARG	4.3
1	F	392	THR	4.3
1	E	171	GLY	4.3
1	C	219	ALA	4.3
1	E	119	ALA	4.3
1	F	113	ALA	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	288	SER	4.3
1	F	132	VAL	4.3
1	F	29	TRP	4.2
1	F	285	ILE	4.2
1	E	3	TRP	4.2
1	B	232	PRO	4.2
1	E	356	LYS	4.2
1	C	340	VAL	4.2
1	D	323	ILE	4.2
1	E	96	ALA	4.2
1	F	255	VAL	4.2
1	E	87	LYS	4.2
1	E	120	ARG	4.2
1	F	307	GLU	4.2
1	E	197	PRO	4.2
1	F	333	LEU	4.2
1	E	387	ASP	4.1
1	E	6	TYR	4.1
1	F	34	GLN	4.1
1	E	391	PRO	4.1
1	F	262	PRO	4.1
1	F	201	GLY	4.1
1	F	5	ASP	4.1
1	E	137	ASP	4.1
1	F	173	ASP	4.1
1	D	95	PHE	4.1
1	D	198	PHE	4.1
1	D	15	LEU	4.1
1	E	392	THR	4.1
1	F	64	HIS	4.1
1	F	81	SER	4.1
1	E	365	LEU	4.0
1	F	311	ALA	4.0
1	F	290	HIS	4.0
1	C	319	PHE	4.0
1	E	248	THR	4.0
1	E	159	LEU	4.0
1	E	277	ALA	4.0
1	E	157	ARG	4.0
1	E	170	ALA	4.0
1	D	260	LYS	4.0
1	E	314	ASP	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	187[A]	ARG	3.9
1	B	224	GLU	3.9
1	E	355	SER	3.9
1	B	198	PHE	3.9
1	F	145	THR	3.9
1	E	158	ASP	3.9
1	F	314	ASP	3.9
1	F	387	ASP	3.9
1	E	114	SER	3.8
1	C	181[A]	THR	3.8
1	E	214	GLN	3.8
1	F	214	GLN	3.8
1	F	109	HIS	3.8
1	E	173	ASP	3.8
1	E	310	LYS	3.8
1	F	241	GLY	3.8
1	F	151	LEU	3.8
1	F	352	LEU	3.8
1	E	81	SER	3.8
1	E	2	ASN	3.8
1	E	249	TRP	3.7
1	F	375	VAL	3.7
1	F	278	VAL	3.7
1	E	315	THR	3.7
1	B	342	ILE	3.7
1	E	167	ALA	3.7
1	E	303	ASP	3.7
1	F	83	GLU	3.7
1	C	286	TYR	3.7
1	E	102	ALA	3.7
1	F	149	PHE	3.7
1	F	216	LYS	3.7
1	D	98	ILE	3.7
1	D	386	ILE	3.7
1	E	278	VAL	3.7
1	F	133	SER	3.6
1	D	387	ASP	3.6
1	E	251	ASP	3.6
1	F	291	GLY	3.6
1	F	251	ASP	3.6
1	F	315	THR	3.6
1	C	230	ASP	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	126	ILE	3.6
1	E	318	LEU	3.6
1	F	268	ILE	3.6
1	E	8	ASN	3.6
1	D	215	LYS	3.6
1	E	84	LEU	3.6
1	E	252	ILE	3.6
1	C	96	ALA	3.5
1	E	75	ALA	3.5
1	E	113	ALA	3.5
1	F	306	PRO	3.5
1	A	226	GLU	3.5
1	D	240	HIS	3.5
1	E	244	GLY	3.5
1	F	194	SER	3.5
1	E	388	ALA	3.5
1	E	245	HIS	3.5
1	D	17	GLY	3.4
1	E	155	GLU	3.4
1	B	218	LYS	3.4
1	E	156	ASP	3.4
1	E	330	VAL	3.4
1	D	1	SER	3.4
1	C	342	ILE	3.4
1	E	117	ALA	3.4
1	F	6	TYR	3.4
1	B	329	VAL	3.4
1	D	372	ILE	3.4
1	F	310	LYS	3.4
1	F	129	THR	3.4
1	F	166	ARG	3.3
1	E	371	LEU	3.3
1	C	94	PHE	3.3
1	F	160	ALA	3.3
1	F	134	SER	3.3
1	F	3	TRP	3.3
1	D	329	VAL	3.3
1	F	370	ASP	3.3
1	E	164	ILE	3.3
1	B	181[A]	THR	3.3
1	F	209	THR	3.3
1	F	118	SER	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	112	ALA	3.3
1	F	111	ASP	3.3
1	C	1	SER	3.3
1	F	120	ARG	3.3
1	E	362	ALA	3.3
1	F	339	ALA	3.3
1	F	95	PHE	3.3
1	F	139	ARG	3.2
1	B	340[A]	VAL	3.2
1	D	218	LYS	3.2
1	F	89	TRP	3.2
1	D	382	LYS	3.2
1	F	69	PRO	3.2
1	F	100	VAL	3.2
1	F	240	HIS	3.2
1	E	77	GLU	3.2
1	E	264	ILE	3.2
1	F	171	GLY	3.2
1	A	1	SER	3.2
1	E	350	ALA	3.2
1	F	282	VAL	3.2
1	F	177	ILE	3.2
1	E	162	SER	3.2
1	B	240[A]	HIS	3.2
1	E	205	THR	3.1
1	B	242[A]	LEU	3.1
1	E	80	LEU	3.1
1	C	314	ASP	3.1
1	F	35	GLN	3.1
1	A	94	PHE	3.1
1	E	154	PRO	3.1
1	F	146	PRO	3.1
1	A	342	ILE	3.1
1	E	108	GLY	3.1
1	F	383	GLU	3.1
1	F	326	GLY	3.1
1	E	163	PHE	3.1
1	A	229	ARG	3.1
1	E	5	ASP	3.1
1	E	40	GLY	3.1
1	E	115	ALA	3.1
1	D	97	PRO	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	97	PRO	3.0
1	F	154	PRO	3.0
1	F	116	GLN	3.0
1	F	281	GLY	3.0
1	B	1	SER	3.0
1	C	223	VAL	3.0
1	E	136	GLU	3.0
1	C	227	GLY	3.0
1	D	250	GLU	3.0
1	F	162	SER	3.0
1	E	279	ASP	3.0
1	F	369	ALA	3.0
1	C	318	LEU	3.0
1	F	297	GLY	3.0
1	E	29	TRP	3.0
1	C	260	LYS	3.0
1	D	343	GLY	3.0
1	E	282	VAL	3.0
1	E	366	LEU	3.0
1	F	277	ALA	3.0
1	E	107	ASP	3.0
1	F	248	THR	3.0
1	F	348	TRP	2.9
1	B	96	ALA	2.9
1	D	197	PRO	2.9
1	F	180	ASP	2.9
1	F	323	ILE	2.9
1	E	184	PHE	2.9
1	B	199	LEU	2.9
1	D	384[A]	LEU	2.9
1	D	339	ALA	2.9
1	C	97	PRO	2.9
1	F	39	PRO	2.9
1	E	181[A]	THR	2.9
1	F	361	VAL	2.9
1	A	372	ILE	2.9
1	F	252	ILE	2.9
1	C	346	TYR	2.9
1	D	266	LYS	2.8
1	F	179	LEU	2.8
1	C	222	GLY	2.8
1	F	289	ASN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	115	ALA	2.8
1	D	253	ASP	2.8
1	C	95	PHE	2.8
1	B	151	LEU	2.8
1	E	79	ASP	2.8
1	F	279	ASP	2.8
1	D	257	SER	2.8
1	E	133	SER	2.8
1	C	323	ILE	2.8
1	E	175	LEU	2.8
1	E	192	THR	2.8
1	C	266	LYS	2.8
1	C	341	GLY	2.8
1	D	241	GLY	2.8
1	E	106	GLN	2.8
1	F	204[A]	LEU	2.8
1	F	110	GLY	2.8
1	C	224	GLU	2.7
1	E	393	ARG	2.7
1	D	79	ASP	2.7
1	A	365	LEU	2.7
1	D	333	LEU	2.7
1	E	179	LEU	2.7
1	E	19	ALA	2.7
1	B	94	PHE	2.7
1	D	144	ASP	2.7
1	F	106	GLN	2.7
1	F	121	THR	2.7
1	F	167	ALA	2.7
1	A	130[A]	LEU	2.7
1	F	22	LEU	2.7
1	E	178	THR	2.7
1	A	98	ILE	2.7
1	B	126	ILE	2.7
1	D	361	VAL	2.7
1	B	29[A]	TRP	2.7
1	D	96	ALA	2.6
1	F	46	ALA	2.6
1	F	206	ASN	2.6
1	E	305	LEU	2.6
1	B	200	ARG	2.6
1	E	288	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	312	SER	2.6
1	F	303	ASP	2.6
1	E	153	TYR	2.6
1	E	202	LEU	2.6
1	E	339	ALA	2.6
1	D	275	ARG	2.6
1	D	149	PHE	2.6
1	D	76	THR	2.6
1	F	205	THR	2.6
1	A	126	ILE	2.6
1	E	297	GLY	2.6
1	F	108	GLY	2.6
1	A	340[A]	VAL	2.6
1	B	16	VAL	2.6
1	C	151	LEU	2.6
1	D	341	GLY	2.6
1	E	78	ARG	2.6
1	C	176	VAL	2.6
1	E	139	ARG	2.5
1	C	101	ILE	2.5
1	E	24	MET	2.5
1	E	35	GLN	2.5
1	F	44	TYR	2.5
1	F	136	GLU	2.5
1	F	267	GLY	2.5
1	F	158	ASP	2.5
1	F	190	ASP	2.5
1	B	233	ARG	2.5
1	D	319	PHE	2.5
1	D	369	ALA	2.5
1	E	65	TRP	2.5
1	C	178	THR	2.5
1	B	346	TYR	2.5
1	E	61	ALA	2.5
1	E	383	GLU	2.5
1	E	21	THR	2.5
1	C	220	HIS	2.5
1	E	204	LEU	2.5
1	F	80	LEU	2.5
1	F	384	LEU	2.5
1	E	31	ALA	2.5
1	E	203	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	334	ALA	2.5
1	F	321	SER	2.5
1	F	355	SER	2.5
1	E	243	PHE	2.5
1	F	155	GLU	2.5
1	D	151	LEU	2.5
1	D	216	LYS	2.5
1	E	275	ARG	2.4
1	F	2	ASN	2.4
1	D	152	TYR	2.4
1	D	295	ALA	2.4
1	F	274	ALA	2.4
1	D	232	PRO	2.4
1	B	365	LEU	2.4
1	E	72	LEU	2.4
1	E	73	MET	2.4
1	F	27	ALA	2.4
1	F	186	TRP	2.4
1	F	249	TRP	2.4
1	E	246	SER	2.4
1	C	343	GLY	2.4
1	C	215	LYS	2.4
1	C	329	VAL	2.4
1	E	100	VAL	2.4
1	F	25	SER	2.4
1	E	347	ALA	2.4
1	E	104	CYS	2.4
1	C	100	VAL	2.4
1	E	380	ASN	2.4
1	A	323	ILE	2.4
1	D	252	ILE	2.4
1	D	314[A]	ASP	2.4
1	F	61	ALA	2.4
1	E	268	ILE	2.3
1	D	318	LEU	2.3
1	E	333	LEU	2.3
1	F	103	LEU	2.3
1	F	67	LEU	2.3
1	F	126	ILE	2.3
1	D	178	THR	2.3
1	F	128	SER	2.3
1	F	31	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	114	SER	2.3
1	F	280	SER	2.2
1	A	29[A]	TRP	2.2
1	A	295	ALA	2.2
1	B	202	LEU	2.2
1	F	117	ALA	2.2
1	B	372	ILE	2.2
1	F	32	HIS	2.2
1	E	341	GLY	2.2
1	F	313	GLY	2.2
1	E	378	TYR	2.2
1	C	321	SER	2.2
1	F	272	ASP	2.2
1	A	225	ALA	2.2
1	E	33	ALA	2.2
1	D	265	LEU	2.2
1	D	254	TRP	2.2
1	D	196	PHE	2.2
1	E	7	GLU	2.2
1	D	208	VAL	2.2
1	E	263	VAL	2.2
1	C	169	GLU	2.2
1	F	30	GLU	2.2
1	B	358	ILE	2.2
1	F	188	PRO	2.2
1	E	129	THR	2.2
1	E	325	THR	2.2
1	F	377	GLY	2.2
1	E	319	PHE	2.2
1	F	271	PRO	2.2
1	F	345	PRO	2.2
1	E	349	GLY	2.2
1	D	158	ASP	2.2
1	C	339	ALA	2.2
1	E	182	TRP	2.2
1	E	280[A]	SER	2.1
1	E	95	PHE	2.1
1	C	290	HIS	2.1
1	E	146	PRO	2.1
1	E	345	PRO	2.1
1	A	287	CYS	2.1
1	F	47	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	44	TYR	2.1
1	A	319	PHE	2.1
1	B	169	GLU	2.1
1	A	375	VAL	2.1
1	F	317	VAL	2.1
1	F	192	THR	2.1
1	B	268	ILE	2.1
1	D	346	TYR	2.1
1	C	288	SER	2.1
1	E	160	ALA	2.1
1	F	371	LEU	2.1
1	E	271	PRO	2.1
1	F	73	MET	2.1
1	C	268	ILE	2.1
1	F	264	ILE	2.1
1	F	346	TYR	2.1
1	D	256	ARG	2.1
1	E	295	ALA	2.1
1	E	316	PRO	2.1
1	F	93	MET	2.1
1	F	147	ALA	2.1
1	E	103	LEU	2.1
1	B	323	ILE	2.1
1	F	161	GLU	2.0
1	A	346	TYR	2.0
1	B	367	ALA	2.0
1	C	291	GLY	2.0
1	D	93	MET	2.0
1	B	361	VAL	2.0
1	D	321	SER	2.0
1	E	67	LEU	2.0
1	F	43	SER	2.0
1	C	254	TRP	2.0
1	F	275	ARG	2.0
1	C	258	ILE	2.0
1	D	14	GLY	2.0
1	E	27	ALA	2.0
1	F	327	ALA	2.0
1	C	187[A]	ARG	2.0
1	E	34	GLN	2.0
1	F	191	LEU	2.0
1	B	186	TRP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	231	ASN	2.0
1	E	267	GLY	2.0
1	F	353	GLY	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
3	SO4	B	406[B]	5/5	0.71	0.23	50,56,56,59	5
3	SO4	A	404[A]	5/5	0.77	0.31	50,56,58,59	5
2	FMN	F	401	31/31	0.80	0.18	74,79,82,82	31
3	SO4	F	402	5/5	0.83	0.14	88,89,89,90	5
3	SO4	E	403	5/5	0.85	0.14	94,95,95,96	5
2	FMN	E	401	31/31	0.86	0.20	74,78,81,81	31
3	SO4	B	404[A]	5/5	0.87	0.23	67,67,68,70	5
3	SO4	C	404	5/5	0.90	0.24	66,66,67,68	5
3	SO4	F	403	5/5	0.93	0.23	72,72,74,74	5
3	SO4	B	405	5/5	0.94	0.26	99,99,101,104	0
3	SO4	A	405	5/5	0.94	0.19	63,64,64,65	5
2	FMN	C	401	31/31	0.96	0.16	29,33,37,39	0
2	FMN	D	401	31/31	0.96	0.10	39,46,51,52	0
3	SO4	E	402	5/5	0.96	0.26	98,98,99,99	0
2	FMN	B	401	31/31	0.97	0.12	23,29,33,36	0
2	FMN	A	401	31/31	0.98	0.15	19,23,26,30	0
3	SO4	D	403	5/5	0.98	0.11	64,64,69,71	0
3	SO4	B	402	5/5	0.99	0.08	38,39,43,43	0
3	SO4	B	403	5/5	0.99	0.09	38,40,44,45	0
3	SO4	C	403	5/5	0.99	0.08	36,42,43,45	0

Continued on next page...

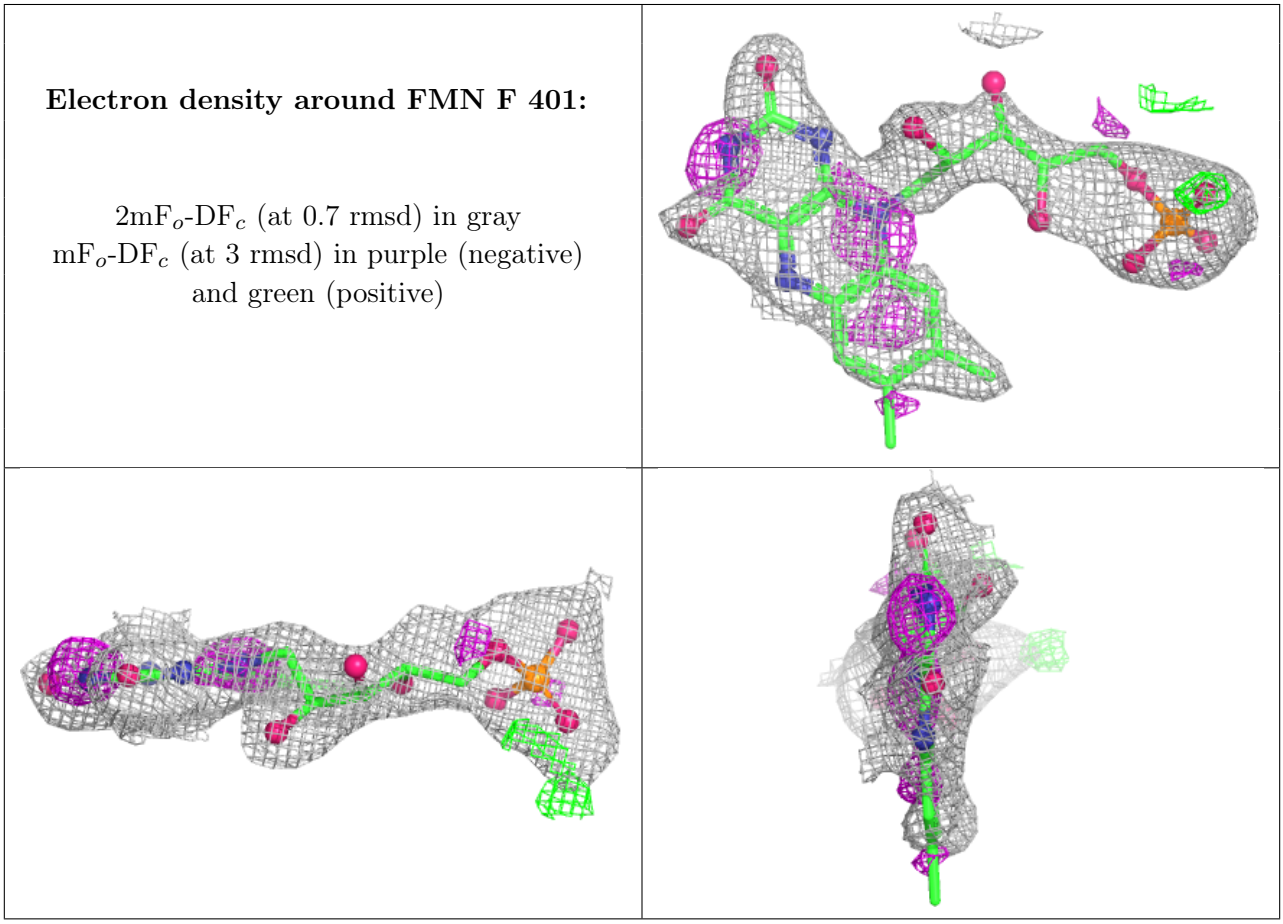
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	403	5/5	0.99	0.12	35,35,39,39	0
3	SO4	D	402	5/5	0.99	0.11	51,51,55,56	0
3	SO4	A	402	5/5	1.00	0.06	30,34,35,37	0
3	SO4	C	402	5/5	1.00	0.08	39,44,46,49	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.

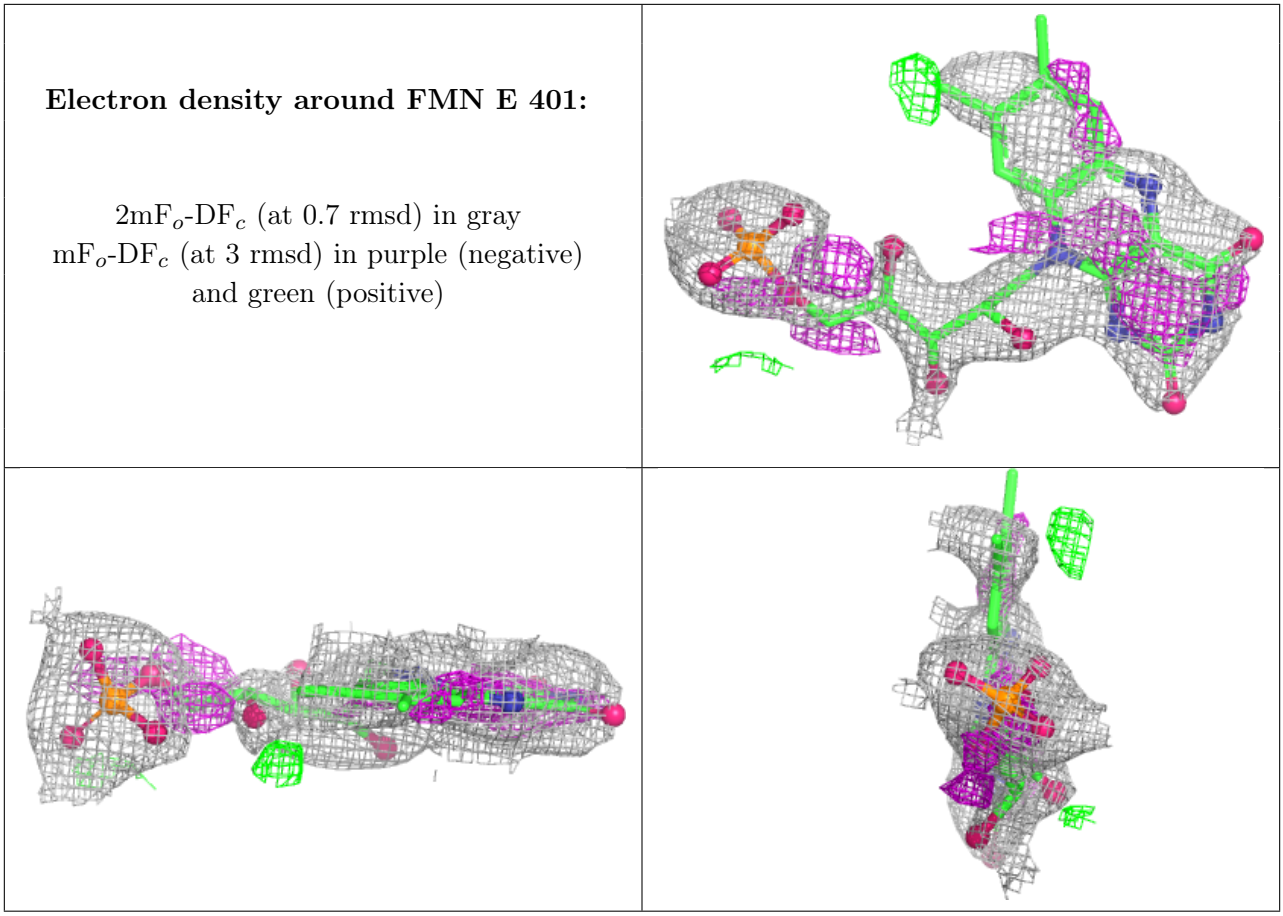
Electron density around FMN F 401:

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



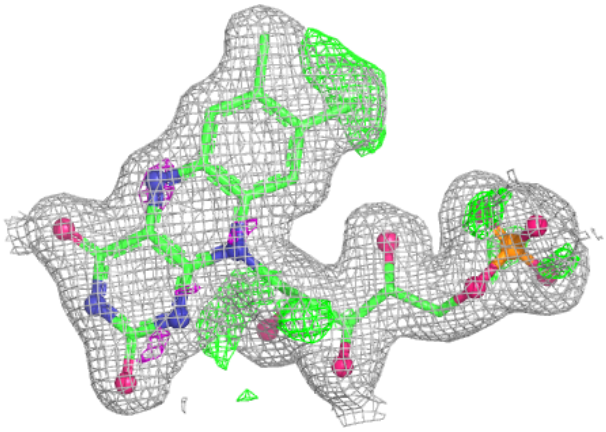
Electron density around FMN E 401:

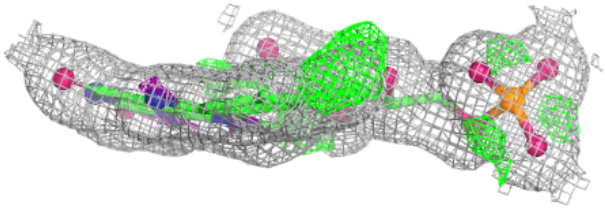
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

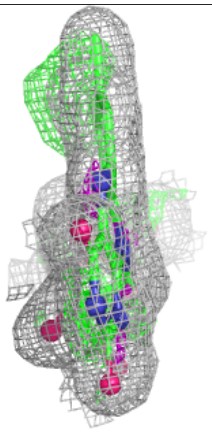


Electron density around FMN C 401:

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

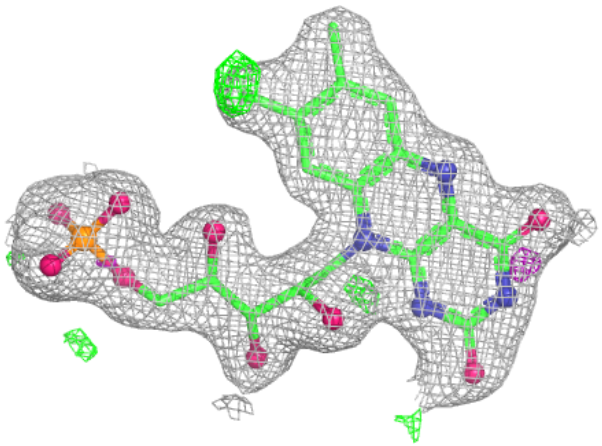


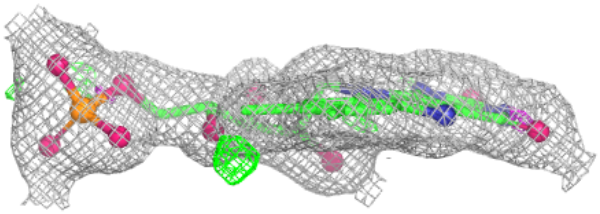


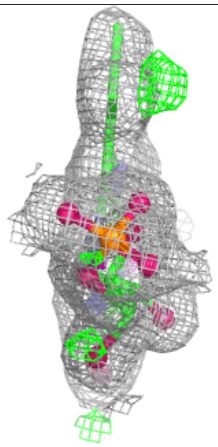


Electron density around FMN D 401:

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

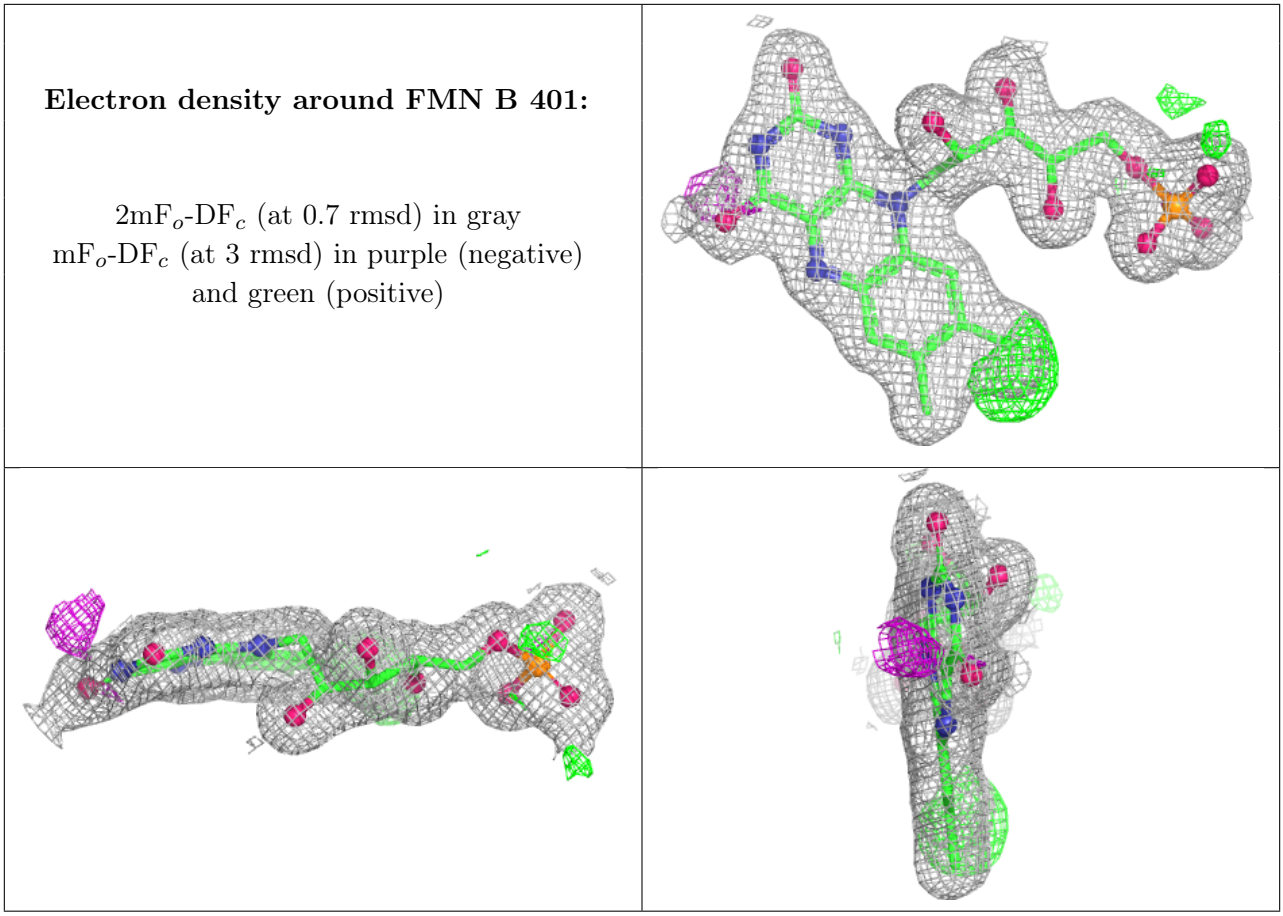






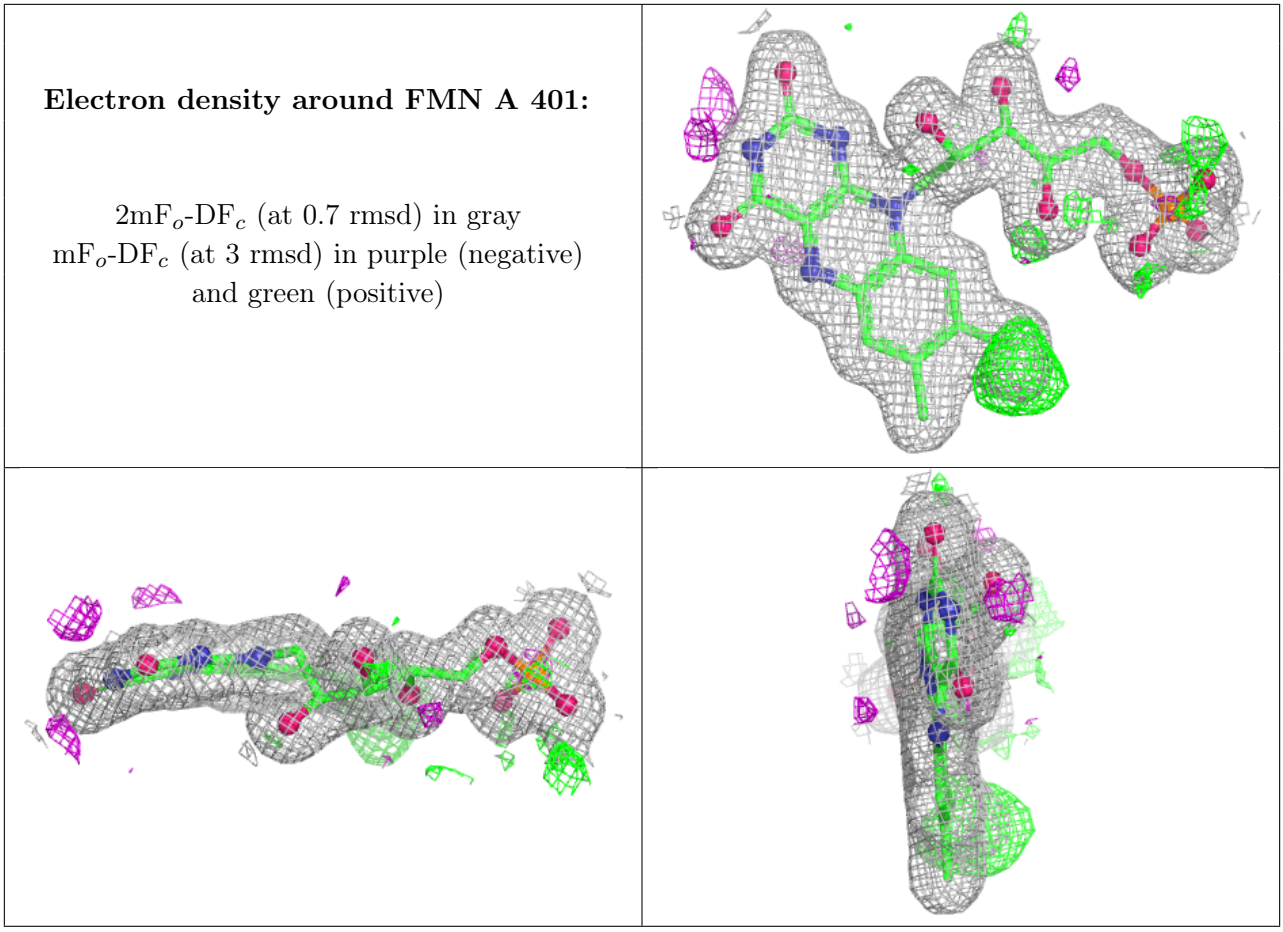
Electron density around FMN B 401:

$2mF_o$-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 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)



6.5 Other polymers

There are no such residues in this entry.