Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 07:37 PM GMT

PDB ID	:	4TMC
Title	:	CRYSTAL STRUCTURE of OLD YELLOW ENZYME from CANDIDA MACEDONIENSIS AKU4588 COMPLEXED with P-HYDROXYBENZALDEHYDE
Authors	:	Horita, S.; Kataoka, M.; Kitamura, N.; Nakagawa, T.; Miyakawa, T.; Ohtsuka, J.; Nagata, K.; Shimizu, S.; Tanokura, M.
Deposited on	:	2014-05-31
Resolution	:	1.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

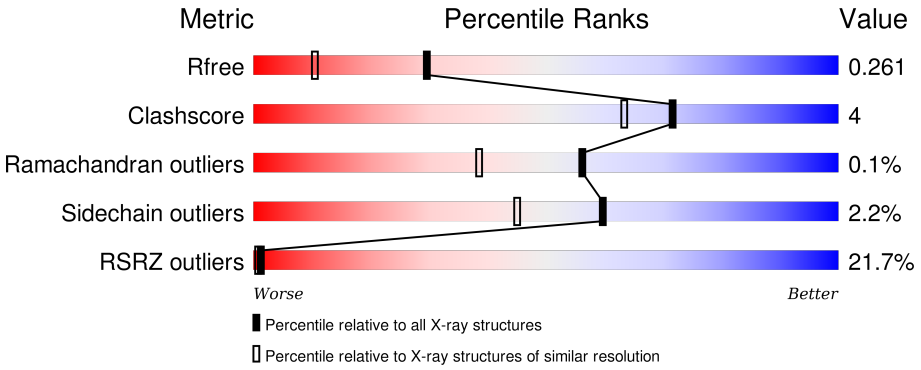
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 1.80 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	403	3% 89% 9%
1	B	403	5% 87% 11%
1	C	403	2% 89% 9%
1	D	403	76% 84% 12%

2 Entry composition

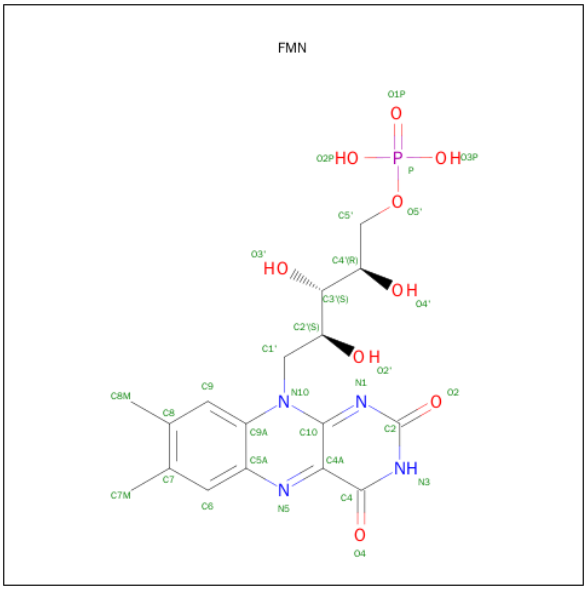
There are 4 unique types of molecules in this entry. The entry contains 14010 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Old yellow enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3209	2055	543	605	6			
1	B	398	Total	C	N	O	S	0	0	0
			3200	2050	542	602	6			
1	C	399	Total	C	N	O	S	0	0	0
			3209	2055	543	605	6			
1	D	396	Total	C	N	O	S	0	0	0
			3182	2038	538	600	6			

- 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		

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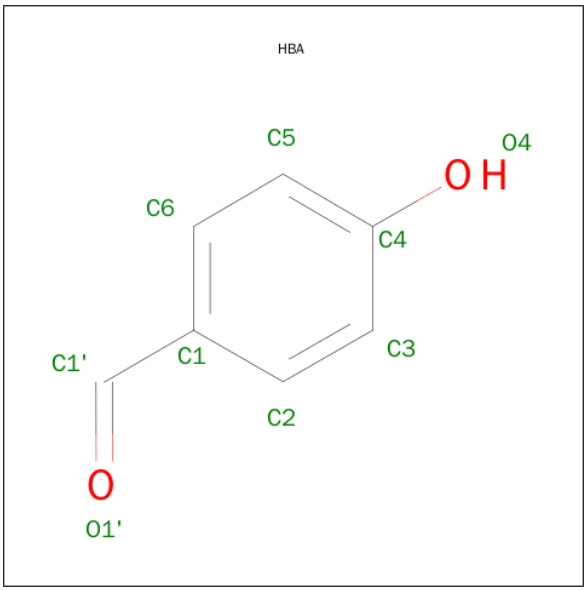
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O P 31 17 4 9 1	0	0
2	D	1	Total C N O P 31 17 4 9 1	0	0

- Molecule 3 is P-HYDROXYBENZALDEHYDE (three-letter code: HBA) (formula: $C_7H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 7 2	0	0
3	B	1	Total C O 9 7 2	0	0
3	C	1	Total C O 9 7 2	0	0
3	D	1	Total C O 9 7 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	310	Total O 310 310	0	0
4	B	254	Total O 254 254	0	0
4	C	280	Total O 280 280	0	0

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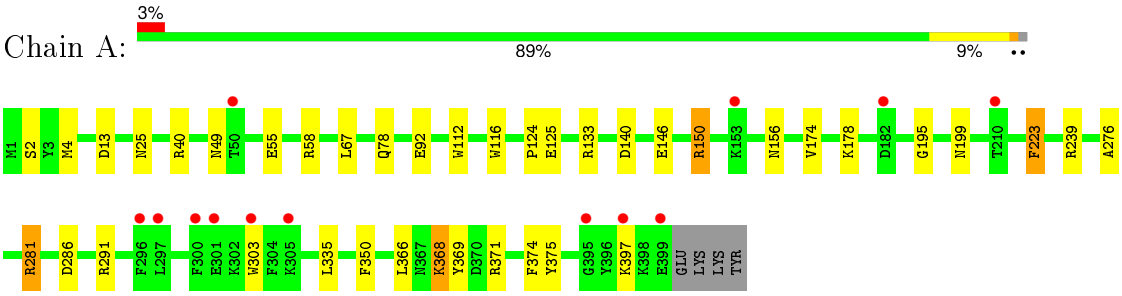
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	206	Total 206	O 206	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

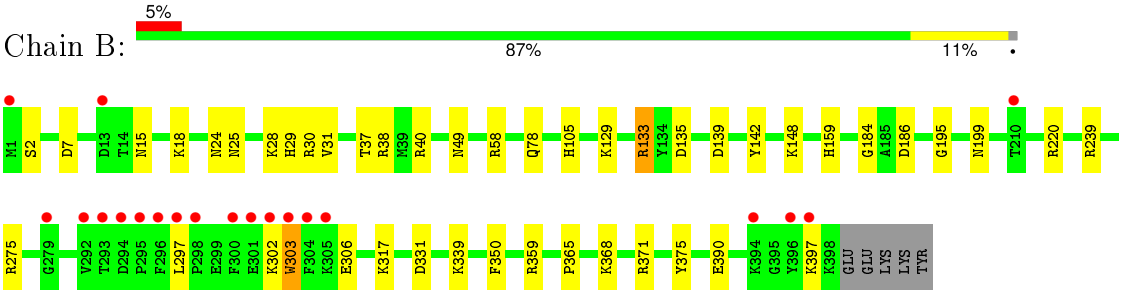
- Molecule 1: Old yellow enzyme

Chain A:



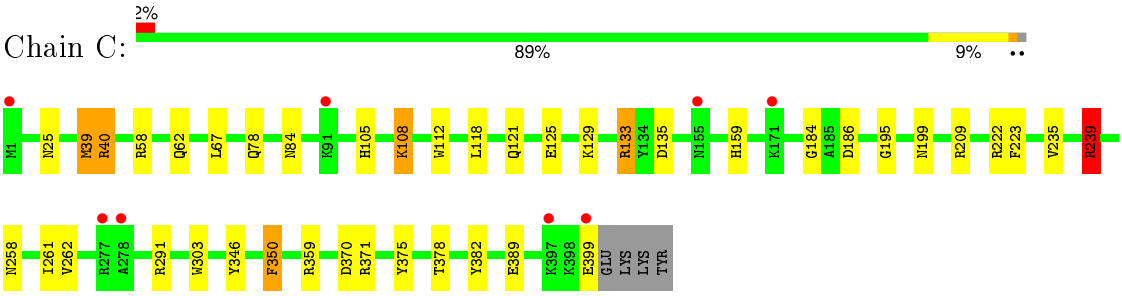
- Molecule 1: Old yellow enzyme

Chain B:



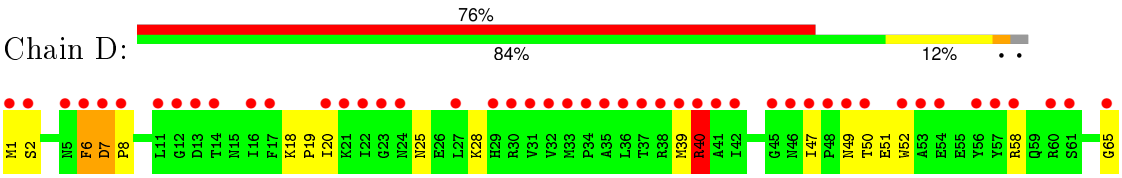
- Molecule 1: Old yellow enzyme

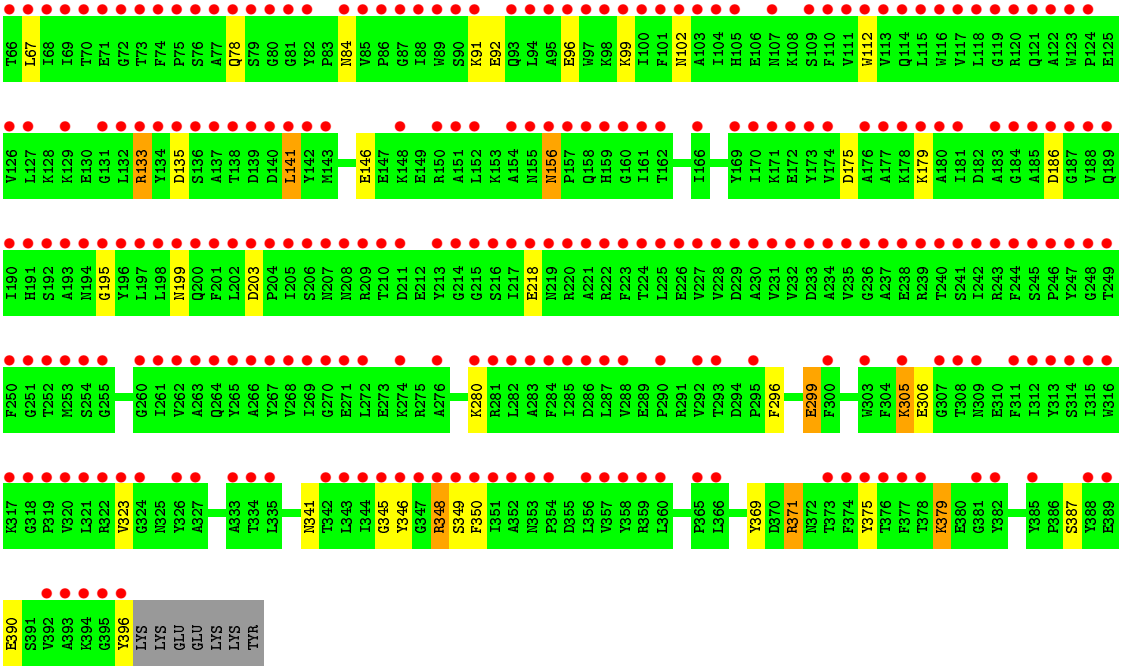
Chain C:



- Molecule 1: Old yellow enzyme

Chain D:




T66 L67 I68 I69 T70 E71 G72 T73 F74 P75 S76 A77 Q78 S79 G80 G81 Y82 P83 N84 V85 P86 G87 I88 W89 S90 K91 E92 Q93 L94 A95 E96 W97 K98 K99 I100 F101 N102 A103 I104 H105 E106 N107 K108 S109 F110 V111 W112 V113 Q114 L115 W116 V117 L118 G119 R120 Q121 A122 W123 P124 E125
V126 L127 K128 K129 E130 G131 L132 R133 Y134 D135 S136 A137 T138 D139 D140 L141 Y142 M143 E146 E147 K148 E149 R150 A151 L152 K153 A154 N155 N156 P157 Q158 H159 G160 I161 T162 I166 Y169 I170 K171 E172 Y173 V174 D175 A176 A177 K178 K179 A180 I181 D182 A183 G184 A185 D186 G187 V188 Q189
I190 H191 S192 A193 N194 G195 Y196 L197 L198 N199 Q200 F201 L202 D203 P204 I205 S206 N207 N208 R209 T210 D211 E212 Y213 G214 G215 S216 I217 E218 N219 R220 A221 R222 F223 T224 L225 E226 V227 V228 D229 A230 V231 V232 D233 A234 V235 G236 A237 E238 R239 T240 S241 I242 R243 F244 S245 P246 Y247 G248 T249
F250 G251 T252 M253 S254 G255 G260 I261 V262 A263 Q264 Y265 A266 Y267 V268 I269 G270 E271 L272 E273 K274 R275 A276 K280 R281 L282 A283 F284 I285 D286 L287 V288 E289 P290 R291 V292 T293 D294 P295 F296 E299 F300 W303 F304 K305 E306 G307 T308 N309 E310 F311 I312 Y313 S314 I315 W316
K317 G318 P319 V320 L321 R322 V323 G324 N325 Y326 A327 A333 T334 L335 N341 T342 L343 I344 G345 Y346 G347 R348 S349 F350 I351 A352 N353 P354 D355 L356 V357 Y358 R359 L360 P365 L366 Y369 D370 R371 N372 T373 F374 Y375 T376 F377 T378 K379 E380 G381 Y382 Y385 P386 S387 Y388 E389
E390 S391 V392 A393 K394 G395 Y396 LYS LYS GLU GLU LYS LYS TYR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.39Å 151.03Å 199.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 1.80 19.95 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.95-1.80) 99.8 (19.95-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.167 , 0.205 0.240 , 0.261	Depositor DCC
R_{free} test set	7395 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 147412 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14010	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, HBA

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	0.97	2/3293 (0.1%)	1.03	9/4463 (0.2%)
1	B	0.97	2/3284 (0.1%)	1.06	19/4451 (0.4%)
1	C	0.95	2/3293 (0.1%)	1.18	21/4463 (0.5%)
1	D	0.89	3/3266 (0.1%)	1.05	13/4429 (0.3%)
All	All	0.94	9/13136 (0.1%)	1.08	62/17806 (0.3%)

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	D	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	389	GLU	CD-OE1	9.07	1.35	1.25
1	D	218	GLU	CD-OE1	7.03	1.33	1.25
1	D	218	GLU	CD-OE2	6.57	1.32	1.25
1	B	133	ARG	CD-NE	-6.40	1.35	1.46
1	B	239	ARG	CD-NE	-6.33	1.35	1.46
1	A	116	TRP	CG-CD1	-5.55	1.28	1.36
1	C	239	ARG	CD-NE	-5.29	1.37	1.46
1	D	40	ARG	CD-NE	-5.28	1.37	1.46
1	A	92	GLU	CD-OE1	5.15	1.31	1.25

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	40	ARG	NE-CZ-NH1	24.27	132.43	120.30
1	C	40	ARG	NE-CZ-NH2	-22.28	109.16	120.30
1	B	133	ARG	NE-CZ-NH2	-20.77	109.91	120.30
1	D	40	ARG	NE-CZ-NH2	-18.41	111.10	120.30
1	D	40	ARG	NE-CZ-NH1	17.81	129.21	120.30
1	A	150	ARG	NE-CZ-NH1	17.19	128.90	120.30
1	B	133	ARG	NE-CZ-NH1	14.85	127.72	120.30
1	C	133	ARG	NE-CZ-NH2	-14.63	112.99	120.30
1	A	150	ARG	NE-CZ-NH2	-13.67	113.46	120.30
1	C	133	ARG	NE-CZ-NH1	13.43	127.02	120.30
1	D	133	ARG	NE-CZ-NH2	-13.27	113.67	120.30
1	C	58	ARG	NE-CZ-NH1	12.45	126.52	120.30
1	C	239	ARG	NE-CZ-NH2	-11.72	114.44	120.30
1	D	133	ARG	NE-CZ-NH1	10.88	125.74	120.30
1	C	58	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	D	348	ARG	NE-CZ-NH2	-9.41	115.60	120.30
1	C	239	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	C	40	ARG	CD-NE-CZ	9.13	136.38	123.60
1	D	348	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	D	40	ARG	CD-NE-CZ	8.40	135.37	123.60
1	A	286	ASP	CB-CG-OD1	7.91	125.42	118.30
1	C	108	LYS	CD-CE-NZ	7.87	129.80	111.70
1	B	133	ARG	CD-NE-CZ	7.46	134.05	123.60
1	D	371	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	239	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	C	40	ARG	CB-CG-CD	7.20	130.32	111.60
1	B	275	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	A	58	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	D	58	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	D	371	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	B	58	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	C	62	GLN	CB-CA-C	-6.70	97.01	110.40
1	C	209	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	B	220	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	C	39	MET	CG-SD-CE	6.23	110.16	100.20
1	A	239	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	D	141	LEU	CB-CG-CD1	6.12	121.39	111.00
1	C	62	GLN	CA-CB-CG	6.04	126.70	113.40
1	B	139	ASP	CB-CG-OD1	6.02	123.71	118.30
1	B	239	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	133	ARG	CB-CG-CD	-5.96	96.10	111.60
1	D	40	ARG	CG-CD-NE	-5.93	99.34	111.80
1	C	371	ARG	NE-CZ-NH1	5.92	123.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	331	ASP	CB-CG-OD1	5.85	123.56	118.30
1	C	222	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	275	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	B	28	LYS	CB-CA-C	5.59	121.58	110.40
1	C	359	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	133	ARG	CA-CB-CG	5.53	125.56	113.40
1	A	335	LEU	CA-CB-CG	5.53	128.02	115.30
1	D	203	ASP	CB-CG-OD1	5.53	123.28	118.30
1	C	399	GLU	N-CA-CB	-5.50	100.70	110.60
1	C	223	PHE	CB-CG-CD1	5.50	124.65	120.80
1	A	286	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	B	58	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	24	ASN	CB-CA-C	-5.27	99.86	110.40
1	A	223	PHE	CB-CG-CD1	5.26	124.48	120.80
1	B	30	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	303	TRP	CA-CB-CG	5.07	123.34	113.70
1	B	390	GLU	CA-CB-CG	5.04	124.48	113.40
1	C	370	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	B	139	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	1	MET	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	3209	0	3138	27	0
1	B	3200	0	3132	26	0
1	C	3209	0	3138	24	0
1	D	3182	0	3106	35	0
2	A	31	0	19	2	0
2	B	31	0	19	2	0
2	C	31	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	31	0	19	3	0
3	A	9	0	5	0	0
3	B	9	0	5	0	0
3	C	9	0	5	0	0
3	D	9	0	5	0	0
4	A	310	0	0	1	0
4	B	254	0	0	3	0
4	C	280	0	0	1	0
4	D	206	0	0	5	0
All	All	14010	0	12610	111	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (111) 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:4:MET:HE3	1:A:366:LEU:HB2	1.37	1.07
1:B:368:LYS:HG3	4:B:823:HOH:O	1.52	1.07
1:D:371:ARG:NH2	4:D:641:HOH:O	2.01	0.93
1:A:55:GLU:HG2	4:A:673:HOH:O	1.75	0.87
1:A:4:MET:CE	1:A:366:LEU:HB2	2.06	0.85
1:A:4:MET:HE3	1:A:366:LEU:CB	2.09	0.82
1:B:133:ARG:HD2	1:B:135:ASP:OD1	1.80	0.82
1:A:4:MET:CE	1:A:366:LEU:CB	2.58	0.81
1:C:78:GLN:HE22	1:C:133:ARG:H	1.31	0.79
1:A:78:GLN:HE22	1:A:133:ARG:H	1.32	0.77
1:D:78:GLN:HE22	1:D:133:ARG:H	1.33	0.76
1:B:195:GLY:H	1:B:199:ASN:HD22	1.36	0.74
1:A:124:PRO:HD2	1:A:150:ARG:HD2	1.70	0.73
1:A:125:GLU:OE1	1:A:150:ARG:HD3	1.88	0.73
1:A:146:GLU:H	1:A:146:GLU:CD	1.92	0.72
1:D:195:GLY:H	1:D:199:ASN:HD22	1.38	0.72
1:C:67:LEU:HD11	1:C:112:TRP:CD1	2.27	0.69
1:B:29:HIS:HD2	1:B:31:VAL:H	1.40	0.68
1:C:40:ARG:HD3	1:C:378:THR:O	1.95	0.67
1:C:25:ASN:HD21	1:C:186:ASP:HB3	1.58	0.66
1:D:18:LYS:HG3	1:D:19:PRO:HD2	1.78	0.66
1:C:195:GLY:H	1:C:199:ASN:HD22	1.44	0.66
1:C:108:LYS:HE3	4:C:759:HOH:O	1.96	0.65
1:D:175:ASP:OD2	1:D:179:LYS:HE2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:VAL:O	1:C:239:ARG:HD3	1.96	0.64
1:C:133:ARG:HD2	1:C:135:ASP:OD1	1.98	0.64
1:D:49:ASN:OD1	1:D:51:GLU:HG3	1.97	0.64
1:D:102:ASN:HB3	4:D:744:HOH:O	1.97	0.64
1:A:195:GLY:H	1:A:199:ASN:HD22	1.44	0.64
1:B:40:ARG:O	1:B:49:ASN:HB2	1.98	0.64
1:B:375:TYR:CE1	2:B:501:FMN:HM72	2.32	0.63
1:B:2:SER:HB2	1:B:397:LYS:O	1.99	0.62
1:C:235:VAL:O	1:C:239:ARG:CD	2.49	0.61
1:A:375:TYR:CE1	2:A:501:FMN:HM72	2.35	0.61
1:B:78:GLN:HE22	1:B:133:ARG:H	1.48	0.61
1:D:195:GLY:H	1:D:199:ASN:ND2	1.99	0.60
1:A:4:MET:CE	1:A:366:LEU:HB3	2.31	0.60
1:B:15:ASN:HD22	1:B:18:LYS:HD2	1.67	0.60
1:B:148:LYS:HE2	4:B:604:HOH:O	2.02	0.60
1:D:299:GLU:OE1	1:D:369:TYR:OH	2.15	0.59
1:A:375:TYR:CZ	2:A:501:FMN:HM72	2.39	0.58
1:B:375:TYR:CZ	2:B:501:FMN:HM72	2.40	0.56
1:C:258:ASN:HB3	1:C:261:ILE:HD13	1.87	0.56
1:D:133:ARG:HD2	1:D:135:ASP:OD1	2.06	0.56
1:C:195:GLY:H	1:C:199:ASN:ND2	2.03	0.56
1:D:348:ARG:HD3	2:D:501:FMN:O1P	2.05	0.56
1:D:280:LYS:CE	4:D:696:HOH:O	2.54	0.56
1:A:40:ARG:O	1:A:49:ASN:HB2	2.06	0.55
1:D:323:VAL:HG22	1:D:345:GLY:HA3	1.88	0.55
1:D:50:THR:OG1	1:D:96:GLU:HB3	2.06	0.55
1:D:40:ARG:O	1:D:49:ASN:HB2	2.07	0.55
1:B:148:LYS:CE	4:B:604:HOH:O	2.56	0.54
1:D:52:TRP:CE2	1:D:379:LYS:HG2	2.43	0.54
1:B:29:HIS:CD2	1:B:31:VAL:H	2.23	0.54
1:A:276:ALA:HB1	1:A:281:ARG:HB2	1.90	0.52
1:B:133:ARG:CD	1:B:135:ASP:OD1	2.56	0.51
1:B:317:LYS:HE2	1:D:306:GLU:HB3	1.92	0.51
1:D:102:ASN:CB	4:D:744:HOH:O	2.54	0.51
1:A:371:ARG:HD2	1:A:374:PHE:CD2	2.46	0.51
1:B:195:GLY:H	1:B:199:ASN:ND2	2.06	0.49
1:B:105:HIS:HE1	1:B:184:GLY:O	1.95	0.49
1:D:375:TYR:CZ	2:D:501:FMN:HM72	2.48	0.49
1:A:276:ALA:CB	1:A:281:ARG:HB2	2.43	0.49
1:C:39:MET:CE	1:C:375:TYR:HB3	2.43	0.48
1:C:261:ILE:HG22	1:C:262:VAL:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:THR:HG21	1:D:99:LYS:HD3	1.95	0.48
1:D:280:LYS:HE2	4:D:696:HOH:O	2.11	0.48
1:C:39:MET:HE3	1:C:375:TYR:HB3	1.94	0.48
1:C:40:ARG:HD2	1:C:382:TYR:CD1	2.49	0.48
1:D:67:LEU:HD11	1:D:112:TRP:CD1	2.48	0.48
1:B:297:LEU:HD13	1:B:302:LYS:HG2	1.96	0.47
1:A:140:ASP:OD1	1:A:140:ASP:N	2.47	0.47
1:B:297:LEU:HD13	1:B:302:LYS:CG	2.45	0.46
1:D:296:PHE:HA	1:D:371:ARG:NH2	2.30	0.46
1:D:20:ILE:CD1	1:D:341:ASN:HD22	2.28	0.46
1:A:125:GLU:CD	1:A:150:ARG:HD3	2.36	0.46
1:B:15:ASN:ND2	1:B:18:LYS:HD2	2.31	0.46
1:A:291:ARG:HA	1:A:303:TRP:CD1	2.51	0.46
1:A:25:ASN:ND2	1:A:112:TRP:HE1	2.13	0.46
1:C:133:ARG:HD3	1:C:159:HIS:CD2	2.52	0.45
1:C:67:LEU:CD1	1:C:112:TRP:CD1	2.98	0.45
1:A:195:GLY:H	1:A:199:ASN:ND2	2.12	0.45
1:A:2:SER:HB2	1:A:397:LYS:O	2.17	0.45
1:C:125:GLU:O	1:C:129:LYS:HD3	2.17	0.44
1:C:235:VAL:O	1:C:239:ARG:HD2	2.18	0.44
1:D:387:SER:OG	1:D:390:GLU:HG3	2.18	0.44
1:C:291:ARG:HA	1:C:303:TRP:CD1	2.53	0.43
1:D:47:ILE:HD12	1:D:92:GLU:HB3	2.00	0.43
1:C:105:HIS:HE1	1:C:184:GLY:O	2.01	0.43
1:D:348:ARG:CD	2:D:501:FMN:O1P	2.67	0.43
1:B:133:ARG:HD3	1:B:159:HIS:CD2	2.53	0.43
1:B:15:ASN:HA	1:B:18:LYS:HG3	2.00	0.43
1:C:39:MET:HA	1:C:84:ASN:O	2.19	0.43
1:A:368:LYS:HD2	1:A:369:TYR:H	1.84	0.43
1:D:6:PHE:CG	1:D:7:ASP:N	2.87	0.43
1:D:305:LYS:HB2	1:D:305:LYS:HE2	1.88	0.42
1:B:25:ASN:HD21	1:B:186:ASP:HB3	1.84	0.42
1:A:67:LEU:HD11	1:A:112:TRP:CD1	2.55	0.42
1:C:40:ARG:HD2	1:C:382:TYR:CG	2.55	0.42
1:B:142:TYR:CE2	1:B:148:LYS:HA	2.55	0.41
1:D:39:MET:HA	1:D:84:ASN:O	2.20	0.41
1:B:37:THR:O	1:B:38:ARG:HD2	2.20	0.41
1:A:4:MET:HE2	1:A:366:LEU:HB3	2.01	0.41
1:A:174:VAL:CG1	1:A:178:LYS:HE3	2.51	0.41
1:D:28:LYS:HG3	1:D:65:GLY:HA3	2.02	0.41
1:B:359:ARG:HD3	1:B:365:PRO:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:TYR:O	1:C:350:PHE:HB2	2.21	0.41
1:D:156:ASN:HA	1:D:156:ASN:HD22	1.72	0.41
1:D:25:ASN:HD21	1:D:186:ASP:HB3	1.86	0.41
1:D:346:TYR:HB3	1:D:349:SER:OG	2.21	0.40
1:D:50:THR:HG1	1:D:96:GLU:HB3	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	397/403 (98%)	386 (97%)	11 (3%)	0	100	100
1	B	396/403 (98%)	382 (96%)	14 (4%)	0	100	100
1	C	397/403 (98%)	385 (97%)	12 (3%)	0	100	100
1	D	394/403 (98%)	379 (96%)	14 (4%)	1 (0%)	46	29
All	All	1584/1612 (98%)	1532 (97%)	51 (3%)	1 (0%)	56	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	6	PHE

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	336/340 (99%)	330 (98%)	6 (2%)	66	54
1	B	335/340 (98%)	328 (98%)	7 (2%)	61	47
1	C	336/340 (99%)	332 (99%)	4 (1%)	78	71
1	D	333/340 (98%)	320 (96%)	13 (4%)	39	21
All	All	1340/1360 (98%)	1310 (98%)	30 (2%)	60	45

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	156	ASN
1	A	223	PHE
1	A	281	ARG
1	A	350	PHE
1	A	368	LYS
1	B	7	ASP
1	B	129	LYS
1	B	303	TRP
1	B	306	GLU
1	B	339	LYS
1	B	350	PHE
1	B	371	ARG
1	C	118	LEU
1	C	121	GLN
1	C	239	ARG
1	C	350	PHE
1	D	2	SER
1	D	7	ASP
1	D	8	PRO
1	D	40	ARG
1	D	91	LYS
1	D	141	LEU
1	D	146	GLU
1	D	156	ASN
1	D	299	GLU
1	D	305	LYS
1	D	350	PHE
1	D	379	LYS
1	D	396	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	46	ASN
1	A	62	GLN
1	A	78	GLN
1	A	107	ASN
1	A	156	ASN
1	A	199	ASN
1	B	15	ASN
1	B	25	ASN
1	B	29	HIS
1	B	46	ASN
1	B	62	GLN
1	B	78	GLN
1	B	199	ASN
1	C	25	ASN
1	C	62	GLN
1	C	78	GLN
1	C	155	ASN
1	C	199	ASN
1	D	15	ASN
1	D	25	ASN
1	D	78	GLN
1	D	156	ASN
1	D	199	ASN
1	D	332	GLN
1	D	341	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FMN	A	501	-	32,33,33	2.02	9 (28%)	34,50,50	2.74	14 (41%)
3	HBA	A	502	-	9,9,9	0.68	0	11,11,11	1.43	2 (18%)
2	FMN	B	501	-	32,33,33	1.79	7 (21%)	34,50,50	2.23	7 (20%)
3	HBA	B	502	-	9,9,9	0.95	0	11,11,11	1.07	0
2	FMN	C	501	-	32,33,33	1.49	4 (12%)	34,50,50	2.71	12 (35%)
3	HBA	C	502	-	9,9,9	0.92	0	11,11,11	1.04	0
2	FMN	D	501	-	32,33,33	1.67	9 (28%)	34,50,50	2.69	10 (29%)
3	HBA	D	502	-	9,9,9	0.84	0	11,11,11	1.12	1 (9%)

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	A	501	-	-	0/18/18/18	0/3/3/3
3	HBA	A	502	-	-	0/2/2/2	0/1/1/1
2	FMN	B	501	-	-	0/18/18/18	0/3/3/3
3	HBA	B	502	-	-	0/2/2/2	0/1/1/1
2	FMN	C	501	-	-	0/18/18/18	0/3/3/3
3	HBA	C	502	-	-	0/2/2/2	0/1/1/1
2	FMN	D	501	-	-	0/18/18/18	0/3/3/3
3	HBA	D	502	-	-	0/2/2/2	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	FMN	C10-N1	-2.70	1.31	1.35
2	A	501	FMN	C6-C5A	-2.60	1.37	1.41
2	B	501	FMN	C6-C5A	-2.19	1.38	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FMN	C9A-N10	2.00	1.41	1.38
2	C	501	FMN	C4-N3	2.03	1.36	1.33
2	A	501	FMN	O2'-C2'	2.05	1.47	1.43
2	D	501	FMN	C8-C7	2.07	1.46	1.41
2	D	501	FMN	O4-C4	2.07	1.29	1.24
2	D	501	FMN	C9A-C5A	2.09	1.47	1.42
2	B	501	FMN	O3'-C3'	2.30	1.48	1.43
2	D	501	FMN	C4-N3	2.47	1.37	1.33
2	A	501	FMN	C4-N3	2.48	1.37	1.33
2	B	501	FMN	C5'-C4'	2.79	1.56	1.51
2	D	501	FMN	C5'-C4'	2.89	1.56	1.51
2	D	501	FMN	P-O5'	2.95	1.68	1.59
2	A	501	FMN	O3'-C3'	3.01	1.50	1.43
2	C	501	FMN	C4-C4A	3.13	1.47	1.41
2	A	501	FMN	C4A-N5	3.24	1.38	1.33
2	B	501	FMN	C8-C7	3.28	1.49	1.41
2	D	501	FMN	C4A-C10	3.38	1.47	1.40
2	B	501	FMN	C9A-C5A	3.53	1.50	1.42
2	D	501	FMN	C4-C4A	3.60	1.48	1.41
2	A	501	FMN	C9A-N10	3.78	1.44	1.38
2	B	501	FMN	C4-C4A	4.11	1.49	1.41
2	A	501	FMN	C5'-C4'	4.13	1.58	1.51
2	A	501	FMN	C4-C4A	4.26	1.49	1.41
2	B	501	FMN	C4A-C10	4.60	1.49	1.40
2	C	501	FMN	C4A-C10	4.78	1.49	1.40
2	A	501	FMN	C4A-C10	5.18	1.50	1.40

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	FMN	C4-C4A-C10	-5.74	116.27	119.94
2	C	501	FMN	C4A-C4-N3	-5.58	116.23	123.52
2	A	501	FMN	C4-C4A-C10	-5.30	116.55	119.94
2	B	501	FMN	C4A-C4-N3	-5.22	116.70	123.52
2	D	501	FMN	C4A-C4-N3	-4.89	117.13	123.52
2	A	501	FMN	C4A-C4-N3	-4.57	117.55	123.52
2	A	501	FMN	C4A-C10-N10	-3.81	117.75	120.52
2	B	501	FMN	C4-C4A-C10	-3.60	117.64	119.94
2	C	501	FMN	C4-C4A-C10	-3.52	117.69	119.94
2	D	501	FMN	N3-C2-N1	-3.44	121.90	127.69
3	A	502	HBA	O1'-C1'-C1	-3.42	113.40	124.60
2	C	501	FMN	N3-C2-N1	-3.07	122.53	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	FMN	O5'-P-O1P	-3.00	99.54	107.08
2	C	501	FMN	C4A-C10-N10	-2.97	118.36	120.52
3	D	502	HBA	O1'-C1'-C1	-2.60	116.07	124.60
2	C	501	FMN	C7M-C7-C8	-2.44	115.49	120.73
2	A	501	FMN	C9A-C5A-N5	-2.28	118.46	122.18
2	B	501	FMN	N3-C2-N1	-2.27	123.86	127.69
3	A	502	HBA	C5-C6-C1	-2.14	118.66	121.29
2	A	501	FMN	N3-C2-N1	-2.11	124.14	127.69
2	C	501	FMN	O2P-P-O5'	-2.06	100.72	106.72
2	A	501	FMN	C6-C5A-N5	2.06	121.49	118.92
2	A	501	FMN	O4'-C4'-C3'	2.14	114.47	108.96
2	C	501	FMN	O3P-P-O2P	2.30	115.90	107.44
2	D	501	FMN	C4A-N5-C5A	2.46	119.63	116.72
2	B	501	FMN	O3P-P-O1P	2.68	119.38	110.63
2	D	501	FMN	C4-C4A-N5	2.75	122.05	118.70
2	C	501	FMN	C5A-C9A-N10	2.80	119.67	117.58
2	D	501	FMN	O3P-P-O2P	2.87	117.97	107.44
2	A	501	FMN	O3'-C3'-C4'	2.91	116.28	108.73
2	D	501	FMN	C5A-C9A-N10	3.23	120.00	117.58
2	A	501	FMN	C1'-N10-C9A	3.25	122.59	118.83
2	C	501	FMN	C1'-N10-C9A	3.42	122.79	118.83
2	C	501	FMN	C4-C4A-N5	3.54	123.00	118.70
2	B	501	FMN	C4-C4A-N5	3.56	123.03	118.70
2	A	501	FMN	C4-C4A-N5	3.63	123.12	118.70
2	A	501	FMN	O2'-C2'-C1'	3.88	119.52	109.93
2	B	501	FMN	C4A-N5-C5A	4.00	121.44	116.72
2	A	501	FMN	C5A-C9A-N10	4.59	121.02	117.58
2	D	501	FMN	C1'-N10-C9A	4.70	124.28	118.83
2	A	501	FMN	C4A-N5-C5A	5.04	122.66	116.72
2	C	501	FMN	C4A-N5-C5A	5.42	123.11	116.72
2	B	501	FMN	C4-N3-C2	7.71	121.59	115.16
2	A	501	FMN	C4-N3-C2	8.41	122.17	115.16
2	C	501	FMN	C4-N3-C2	9.49	123.07	115.16
2	D	501	FMN	C4-N3-C2	9.99	123.49	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FMN	2	0
2	B	501	FMN	2	0
2	D	501	FMN	3	0

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	399/403 (99%)	-0.13	13 (3%) 50 44	14, 21, 35, 49	0
1	B	398/403 (98%)	0.11	20 (5%) 32 27	15, 24, 45, 63	0
1	C	399/403 (99%)	0.05	8 (2%) 68 64	16, 24, 39, 50	0
1	D	396/403 (98%)	3.98	305 (77%) 0 0	49, 83, 121, 145	0
All	All	1592/1612 (98%)	1.00	346 (21%) 1 1	14, 26, 104, 145	0

All (346) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	97	TRP	13.7
1	D	134	TYR	12.5
1	D	197	LEU	12.1
1	D	201	PHE	11.5
1	D	136	SER	11.2
1	D	173	TYR	9.9
1	D	118	LEU	9.5
1	D	73	THR	9.5
1	D	88	ILE	9.4
1	D	237	ALA	9.3
1	D	87	GLY	9.1
1	D	74	PHE	8.9
1	D	225	LEU	8.8
1	D	86	PRO	8.7
1	D	101	PHE	8.6
1	D	198	LEU	8.6
1	D	223	PHE	8.5
1	D	228	VAL	8.5
1	D	285	ILE	8.4
1	D	213	TYR	8.4
1	D	41	ALA	8.3

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Mol	Chain	Res	Type	RSRZ
1	D	196	TYR	8.3
1	D	100	ILE	8.2
1	D	267	TYR	8.2
1	D	142	TYR	8.1
1	D	48	PRO	8.1
1	D	316	TRP	8.1
1	D	272	LEU	8.0
1	D	227	VAL	8.0
1	D	224	THR	7.9
1	D	240	THR	7.8
1	D	115	LEU	7.8
1	D	85	VAL	7.8
1	D	113	VAL	7.8
1	D	122	ALA	7.7
1	D	190	ILE	7.6
1	D	117	VAL	7.5
1	D	202	LEU	7.5
1	D	269	ILE	7.4
1	D	188	VAL	7.4
1	D	282	LEU	7.4
1	D	244	PHE	7.4
1	D	127	LEU	7.2
1	D	377	PHE	7.1
1	D	124	PRO	7.1
1	D	161	ILE	7.1
1	B	303	TRP	7.1
1	D	120	ARG	7.0
1	D	56	TYR	7.0
1	D	382	TYR	7.0
1	D	283	ALA	6.9
1	D	180	ALA	6.9
1	D	199	ASN	6.9
1	D	119	GLY	6.9
1	D	242	ILE	6.8
1	B	300	PHE	6.8
1	D	392	VAL	6.8
1	D	40	ARG	6.8
1	D	170	ILE	6.7
1	D	137	ALA	6.6
1	D	166	ILE	6.5
1	D	174	VAL	6.5
1	D	116	TRP	6.5

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Mol	Chain	Res	Type	RSRZ
1	D	231	VAL	6.4
1	D	288	VAL	6.4
1	D	111	VAL	6.3
1	D	356	LEU	6.3
1	D	89	TRP	6.3
1	D	75	PRO	6.2
1	D	158	GLN	6.2
1	D	151	ALA	6.2
1	D	79	SER	6.2
1	D	268	VAL	6.2
1	D	221	ALA	6.2
1	D	287	LEU	6.1
1	D	321	LEU	6.0
1	D	350	PHE	6.0
1	D	351	ILE	6.0
1	D	232	VAL	6.0
1	D	16	ILE	6.0
1	D	343	LEU	5.9
1	D	209	ARG	5.9
1	D	323	VAL	5.8
1	D	320	VAL	5.8
1	D	315	ILE	5.8
1	D	270	GLY	5.7
1	D	169	TYR	5.7
1	D	344	ILE	5.6
1	D	135	ASP	5.6
1	D	72	GLY	5.6
1	D	57	TYR	5.6
1	D	77	ALA	5.6
1	D	67	LEU	5.5
1	D	185	ALA	5.5
1	D	263	ALA	5.5
1	D	200	GLN	5.5
1	D	214	GLY	5.5
1	D	193	ALA	5.4
1	D	22	ILE	5.4
1	D	206	SER	5.4
1	D	192	SER	5.4
1	D	217	ILE	5.4
1	D	346	TYR	5.3
1	D	36	LEU	5.3
1	D	141	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	D	284	PHE	5.3
1	D	121	GLN	5.3
1	D	47	ILE	5.2
1	D	266	ALA	5.2
1	D	132	LEU	5.2
1	D	345	GLY	5.2
1	D	80	GLY	5.2
1	D	324	GLY	5.2
1	D	374	PHE	5.1
1	D	210	THR	5.1
1	D	195	GLY	5.1
1	D	312	ILE	5.1
1	D	27	LEU	5.0
1	D	181	ILE	5.0
1	D	123	TRP	4.9
1	B	305	LYS	4.9
1	D	23	GLY	4.9
1	B	298	PRO	4.9
1	D	176	ALA	4.9
1	D	347	GLY	4.9
1	D	230	ALA	4.9
1	B	304	PHE	4.8
1	D	253	MET	4.8
1	D	250	PHE	4.8
1	D	31	VAL	4.8
1	D	205	ILE	4.8
1	D	222	ARG	4.8
1	D	143	MET	4.8
1	D	81	GLY	4.7
1	D	104	ILE	4.7
1	D	241	SER	4.7
1	D	109	SER	4.7
1	D	207	ASN	4.7
1	D	319	PRO	4.7
1	D	236	GLY	4.6
1	D	78	GLN	4.6
1	D	70	THR	4.6
1	D	138	THR	4.6
1	D	220	ARG	4.5
1	D	261	ILE	4.5
1	D	39	MET	4.5
1	D	265	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	191	HIS	4.5
1	D	94	LEU	4.4
1	D	37	THR	4.4
1	D	251	GLY	4.4
1	D	53	ALA	4.2
1	D	46	ASN	4.2
1	D	112	TRP	4.2
1	D	318	GLY	4.2
1	D	160	GLY	4.1
1	D	82	TYR	4.1
1	D	247	TYR	4.1
1	D	140	ASP	4.1
1	D	203	ASP	4.1
1	D	352	ALA	4.1
1	D	235	VAL	4.0
1	D	389	GLU	4.0
1	D	32	VAL	4.0
1	D	126	VAL	3.9
1	D	358	TYR	3.9
1	D	262	VAL	3.9
1	D	292	VAL	3.9
1	D	66	THR	3.9
1	D	396	TYR	3.9
1	D	187	GLY	3.9
1	D	239	ARG	3.9
1	D	177	ALA	3.9
1	D	314	SER	3.9
1	D	68	ILE	3.9
1	D	1	MET	3.8
1	D	281	ARG	3.8
1	D	360	LEU	3.8
1	D	42	ILE	3.8
1	B	292	VAL	3.8
1	D	114	GLN	3.8
1	D	226	GLU	3.8
1	D	255	GLY	3.8
1	D	133	ARG	3.8
1	D	229	ASP	3.7
1	D	103	ALA	3.7
1	D	69	ILE	3.7
1	D	49	ASN	3.7
1	D	110	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	373	THR	3.7
1	B	297	LEU	3.7
1	B	294	ASP	3.6
1	D	157	PRO	3.6
1	D	183	ALA	3.6
1	D	381	GLY	3.6
1	B	1	MET	3.6
1	B	296	PHE	3.6
1	D	342	THR	3.6
1	D	35	ALA	3.6
1	D	234	ALA	3.6
1	D	353	ASN	3.6
1	D	395	GLY	3.6
1	D	156	ASN	3.5
1	D	393	ALA	3.5
1	D	20	ILE	3.5
1	B	301	GLU	3.5
1	D	95	ALA	3.5
1	D	93	GLN	3.5
1	D	219	ASN	3.5
1	D	159	HIS	3.5
1	D	349	SER	3.5
1	D	60	ARG	3.5
1	D	264	GLN	3.5
1	D	311	PHE	3.5
1	D	50	THR	3.5
1	D	5	ASN	3.4
1	D	171	LYS	3.4
1	D	260	GLY	3.4
1	D	375	TYR	3.4
1	D	152	LEU	3.4
1	D	245	SER	3.4
1	D	376	THR	3.4
1	D	303	TRP	3.4
1	D	378	THR	3.4
1	D	17	PHE	3.4
1	B	13	ASP	3.4
1	D	211	ASP	3.4
1	D	61	SER	3.3
1	D	194	ASN	3.3
1	D	300	PHE	3.3
1	D	254	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	397	LYS	3.3
1	D	357	VAL	3.3
1	D	33	MET	3.3
1	D	246	PRO	3.3
1	D	326	TYR	3.3
1	D	385	TYR	3.3
1	D	7	ASP	3.2
1	D	139	ASP	3.2
1	D	178	LYS	3.2
1	D	105	HIS	3.2
1	D	313	TYR	3.2
1	D	184	GLY	3.2
1	D	218	GLU	3.2
1	D	271	GLU	3.1
1	D	365	PRO	3.1
1	D	348	ARG	3.1
1	D	148	LYS	3.1
1	D	216	SER	3.1
1	D	154	ALA	3.1
1	D	354	PRO	3.1
1	D	38	ARG	3.1
1	D	248	GLY	3.0
1	B	295	PRO	3.0
1	D	2	SER	3.0
1	D	65	GLY	3.0
1	D	34	PRO	3.0
1	D	322	ARG	2.9
1	C	278	ALA	2.9
1	D	162	THR	2.9
1	D	335	LEU	2.9
1	A	399	GLU	2.9
1	A	50	THR	2.9
1	C	1	MET	2.9
1	D	13	ASP	2.9
1	A	210	THR	2.8
1	D	333	ALA	2.8
1	D	76	SER	2.8
1	D	189	GLN	2.8
1	D	238	GLU	2.8
1	D	249	THR	2.7
1	D	208	ASN	2.7
1	D	8	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	11	LEU	2.7
1	D	366	LEU	2.7
1	A	395	GLY	2.7
1	C	397	LYS	2.7
1	D	274	LYS	2.7
1	D	215	GLY	2.7
1	D	286	ASP	2.7
1	D	98	LYS	2.7
1	D	14	THR	2.7
1	D	308	THR	2.7
1	C	155	ASN	2.6
1	D	71	GLU	2.6
1	D	243	ARG	2.6
1	D	309	ASN	2.6
1	D	21	LYS	2.6
1	A	303	TRP	2.6
1	D	276	ALA	2.6
1	D	6	PHE	2.5
1	D	12	GLY	2.5
1	D	129	LYS	2.5
1	D	107	ASN	2.5
1	D	155	ASN	2.5
1	D	96	GLU	2.5
1	D	186	ASP	2.5
1	D	204	PRO	2.5
1	D	334	THR	2.5
1	B	302	LYS	2.5
1	C	277	ARG	2.5
1	D	29	HIS	2.5
1	D	102	ASN	2.5
1	D	24	ASN	2.4
1	D	388	TYR	2.4
1	D	45	GLY	2.4
1	D	90	SER	2.4
1	D	305	LYS	2.4
1	D	233	ASP	2.4
1	D	290	PRO	2.4
1	D	150	ARG	2.4
1	D	54	GLU	2.4
1	D	327	ALA	2.3
1	D	295	PRO	2.3
1	A	297	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	91	LYS	2.3
1	D	99	LYS	2.3
1	D	84	ASN	2.3
1	D	359	ARG	2.3
1	A	153	LYS	2.3
1	C	91	LYS	2.3
1	A	305	LYS	2.3
1	D	280	LYS	2.3
1	D	307	GLY	2.2
1	D	252	THR	2.2
1	D	179	LYS	2.2
1	A	397	LYS	2.2
1	A	300	PHE	2.2
1	C	399	GLU	2.2
1	B	279	GLY	2.2
1	D	131	GLY	2.2
1	D	317	LYS	2.2
1	D	30	ARG	2.2
1	D	394	LYS	2.2
1	B	210	THR	2.1
1	B	396	TYR	2.1
1	D	172	GLU	2.1
1	D	52	TRP	2.1
1	B	394	LYS	2.1
1	D	58	ARG	2.1
1	A	182	ASP	2.1
1	B	293	THR	2.0
1	D	293	THR	2.0
1	A	296	PHE	2.0
1	C	171	LYS	2.0
1	A	301	GLU	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 carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	HBA	A	502	9/9	0.89	0.16	1.43	21,23,26,35	0
2	FMN	B	501	31/31	0.90	0.16	0.99	22,25,29,30	0
3	HBA	B	502	9/9	0.84	0.18	0.81	22,31,38,48	0
3	HBA	C	502	9/9	0.91	0.11	0.47	19,21,27,32	0
2	FMN	A	501	31/31	0.94	0.10	0.42	17,20,22,22	0
2	FMN	C	501	31/31	0.96	0.08	-0.45	17,19,21,22	0
3	HBA	D	502	9/9	0.92	0.14	-2.02	21,22,28,33	0
2	FMN	D	501	31/31	0.93	0.10	-3.73	19,22,28,30	0

6.5 Other polymers

There are no such residues in this entry.