Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 07:37 PM GMT

PDB ID	:	4TMB
Title	:	CRYSTAL STRUCTURE of OLD YELLOW ENZYME from CANDIDA MACEDONIENSIS AKU4588
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:

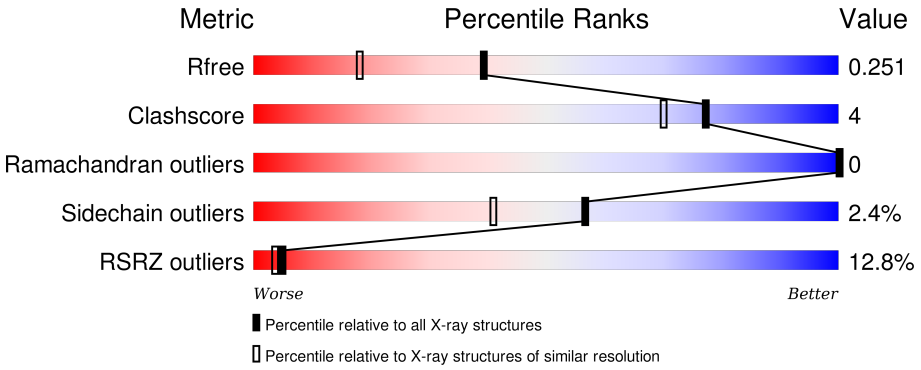
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	2% 87% 9% • •
1	B	403	86% 5% • 7%
1	C	403	2% 86% 8% • 5%
1	D	403	43% 87% 7% • 5%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FMN	A	501	-	-	-	X
2	FMN	B	501	-	-	-	X
2	FMN	C	501	-	-	-	X

2 Entry composition

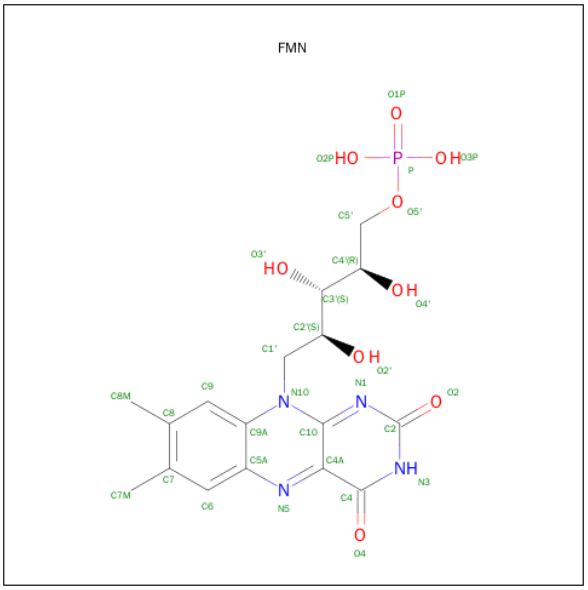
There are 3 unique types of molecules in this entry. The entry contains 13296 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	390	Total	C	N	O	S	0	0	0
			3138	2010	531	592	5			
1	B	374	Total	C	N	O	S	0	0	0
			2991	1910	509	567	5			
1	C	381	Total	C	N	O	S	0	0	0
			3044	1944	518	576	6			
1	D	383	Total	C	N	O	S	0	0	0
			3062	1955	521	580	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	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is water.

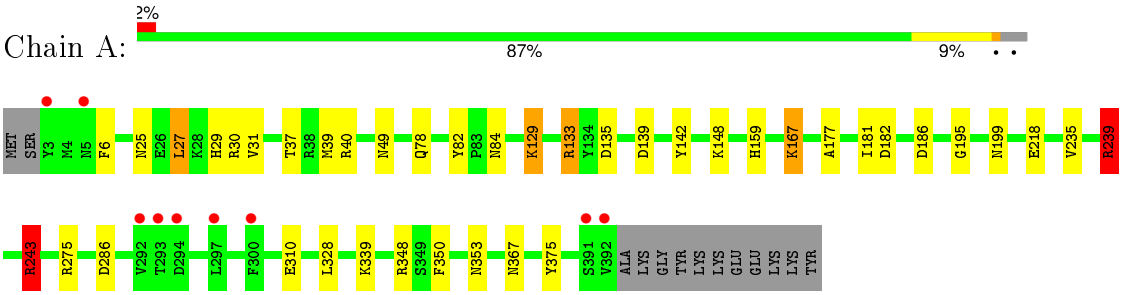
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	247	Total	O	0	0
			247	247		
3	B	263	Total	O	0	0
			263	263		
3	C	178	Total	O	0	0
			178	178		
3	D	249	Total	O	0	0
			249	249		

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.

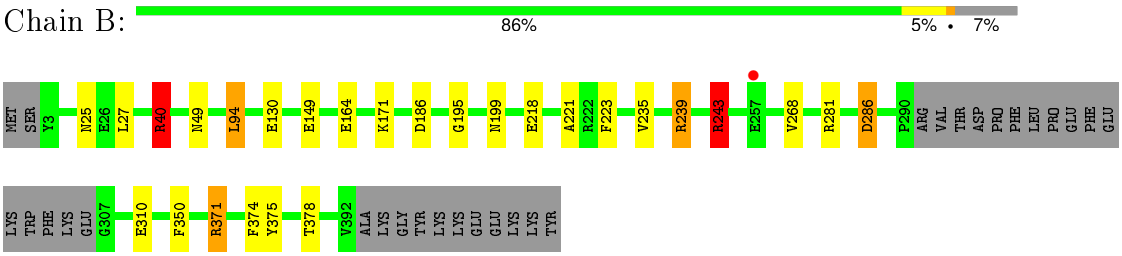
- Molecule 1: Old yellow enzyme

Chain A:



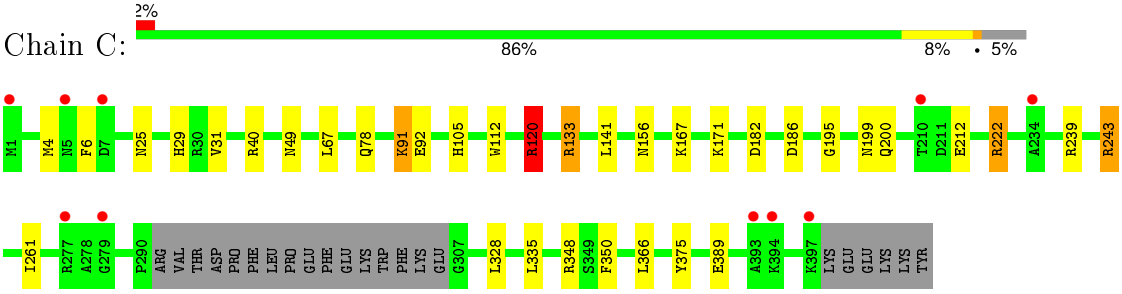
- Molecule 1: Old yellow enzyme

Chain B:



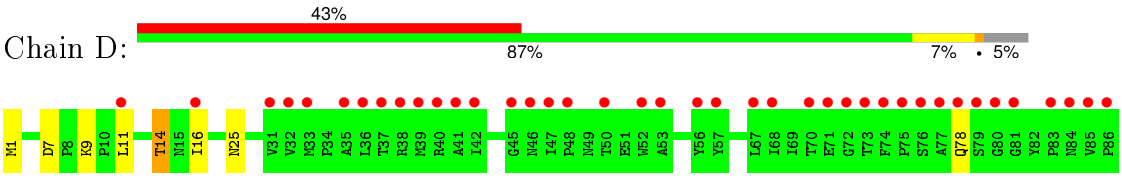
- Molecule 1: Old yellow enzyme

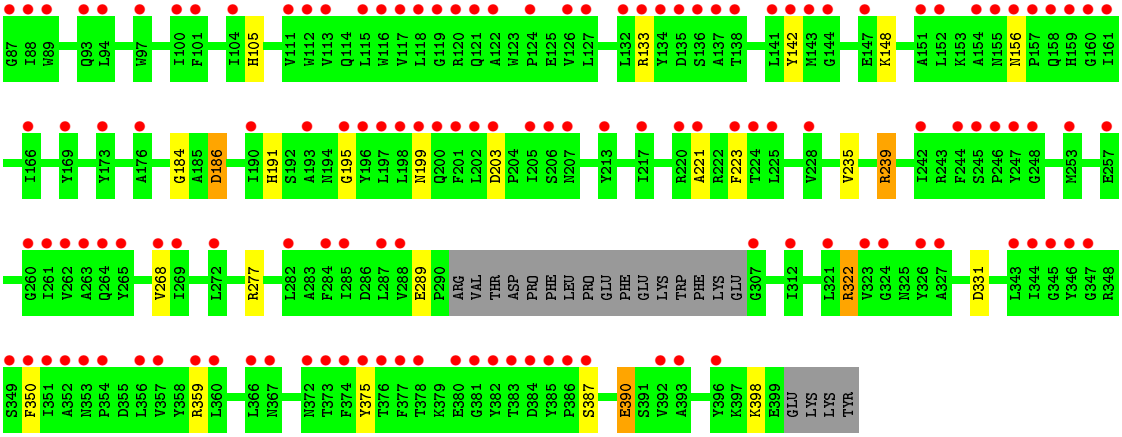
Chain C:



- Molecule 1: Old yellow enzyme

Chain D:




G87 I88 W89 Q93 L94 W97 I100 F101 I104 H105 V111 W112 V113 Q114 L115 W116 V117 L118 G119 R120 Q121 A122 W123 P124 E125 V126 L127 L132 R133 Y134 D135 S136 A137 T138 L141 Y142 M143 G144 E147 K148 A151 L152 K153 A154 N155 N156 P157 Q158 H159 G160 I161
I166 Y169 Y173 A176 G184 A185 D186 I190 H191 S192 A193 N194 G195 Y196 L197 L198 N199 Q200 F201 L202 D203 P204 I205 S206 N207 Y213 I217 R220 A221 R222 F223 T224 L225 V228 V235 R239 I242 R243 F244 S245 P246 Y247 G248 N253 E257
G260 I261 V262 A263 Q264 Y265 V268 I269 L272 R277 L282 A283 F284 I285 D286 L287 V288 E289 P290 ARG VAL THR ASP PRO PHE LEU PRO GLU PHE GLU LYS TRP PHE LYS GLU G307 I312 L321 R322 V323 G324 N325 Y326 A327 D331 L343 I344 G345 Y346 G347 R348
S349 F350 I351 A352 N353 P354 D355 L356 V357 Y358 R359 L360 L366 N367 N372 T373 F374 Y375 T376 F377 T378 K379 E380 G381 Y382 T383 D384 Y385 P386 S387 E390 S391 V392 A393 Y396 K397 K398 E399 GLU LYS LYS TYR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	287.51Å 59.62Å 100.29Å 90.00° 109.89° 90.00°	Depositor
Resolution (Å)	19.82 – 1.80 19.82 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.82-1.80) 99.0 (19.82-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.98 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.172 , 0.210 0.226 , 0.251	Depositor DCC
R_{free} test set	7432 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	17.1	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.5	EDS
Estimated twinning fraction	0.015 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 146754 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13296	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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

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	4/3221 (0.1%)	1.13	13/4370 (0.3%)
1	B	1.03	2/3066 (0.1%)	1.15	17/4158 (0.4%)
1	C	0.87	1/3120 (0.0%)	1.02	10/4228 (0.2%)
1	D	0.97	4/3138 (0.1%)	1.04	8/4251 (0.2%)
All	All	0.96	11/12545 (0.1%)	1.08	48/17007 (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	B	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	322	ARG	CD-NE	-8.44	1.32	1.46
1	A	218	GLU	CD-OE1	6.92	1.33	1.25
1	A	218	GLU	CD-OE2	6.23	1.32	1.25
1	D	387	SER	CB-OG	6.06	1.50	1.42
1	B	149	GLU	CG-CD	5.65	1.60	1.51
1	D	322	ARG	CZ-NH2	-5.61	1.25	1.33
1	A	133	ARG	CD-NE	-5.60	1.36	1.46
1	B	243	ARG	CD-NE	-5.38	1.37	1.46
1	C	120	ARG	CD-NE	-5.08	1.37	1.46
1	A	239	ARG	CD-NE	-5.05	1.37	1.46
1	D	390	GLU	CD-OE2	-5.01	1.20	1.25

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	133	ARG	NE-CZ-NH2	-21.31	109.64	120.30
1	B	40	ARG	NE-CZ-NH2	-21.11	109.75	120.30
1	D	322	ARG	NE-CZ-NH2	-18.66	110.97	120.30
1	D	322	ARG	NE-CZ-NH1	17.80	129.20	120.30
1	C	120	ARG	NE-CZ-NH2	-16.75	111.93	120.30
1	A	243	ARG	NE-CZ-NH1	16.44	128.52	120.30
1	B	40	ARG	NE-CZ-NH1	15.59	128.10	120.30
1	A	239	ARG	NE-CZ-NH2	-15.58	112.51	120.30
1	C	120	ARG	NE-CZ-NH1	15.46	128.03	120.30
1	A	133	ARG	NE-CZ-NH1	15.22	127.91	120.30
1	B	40	ARG	CD-NE-CZ	13.96	143.14	123.60
1	A	239	ARG	NE-CZ-NH1	13.32	126.96	120.30
1	B	40	ARG	CG-CD-NE	-12.05	86.49	111.80
1	A	243	ARG	NE-CZ-NH2	-12.01	114.29	120.30
1	D	239	ARG	NE-CZ-NH1	10.99	125.79	120.30
1	C	120	ARG	CB-CG-CD	10.56	139.04	111.60
1	B	40	ARG	CB-CG-CD	10.12	137.91	111.60
1	D	239	ARG	NE-CZ-NH2	-9.67	115.47	120.30
1	B	243	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	B	281	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	275	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	B	94	LEU	CA-CB-CG	-7.13	98.90	115.30
1	A	133	ARG	CD-NE-CZ	7.03	133.44	123.60
1	B	239	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	239	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	C	222	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	B	223	PHE	CB-CG-CD1	6.75	125.53	120.80
1	D	203	ASP	CB-CG-OD1	6.33	124.00	118.30
1	C	120	ARG	CD-NE-CZ	6.31	132.43	123.60
1	B	223	PHE	CB-CG-CD2	-6.28	116.40	120.80
1	B	27	LEU	CB-CG-CD1	6.12	121.41	111.00
1	C	239	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	C	182	ASP	CB-CG-OD1	5.82	123.53	118.30
1	A	27	LEU	CB-CG-CD1	5.79	120.84	111.00
1	B	243	ARG	CB-CG-CD	-5.72	96.74	111.60
1	A	30	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	D	277	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	C	133	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	243	ARG	CG-CD-NE	5.39	123.11	111.80
1	A	82	TYR	CB-CG-CD1	5.36	124.22	121.00
1	A	139	ASP	CB-CG-OD1	5.27	123.05	118.30
1	C	348	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	218	GLU	OE1-CD-OE2	5.22	129.56	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	186	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	243	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	D	359	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	286	ASP	CB-CG-OD1	5.07	122.86	118.30
1	B	281	ARG	NE-CZ-NH2	-5.07	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	40	ARG	Sidechain

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	3138	0	3059	26	0
1	B	2991	0	2919	21	0
1	C	3044	0	2979	24	0
1	D	3062	0	2998	18	0
2	A	31	0	19	3	0
2	B	31	0	19	4	0
2	C	31	0	19	4	0
2	D	31	0	19	1	0
3	A	247	0	0	1	0
3	B	263	0	0	3	0
3	C	178	0	0	8	0
3	D	249	0	0	1	0
All	All	13296	0	12031	90	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 (90) 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:C:120:ARG:HD3	3:C:617:HOH:O	1.51	1.07
1:A:353:ASN:HD21	1:A:367:ASN:H	1.15	0.94
1:A:133:ARG:HD2	1:A:135:ASP:OD1	1.77	0.84
1:C:212:GLU:O	1:C:222:ARG:NH1	2.11	0.83
1:C:120:ARG:CD	3:C:617:HOH:O	2.18	0.81
1:C:375:TYR:CE1	2:C:501:FMN:HM72	2.18	0.79
1:A:78:GLN:HE22	1:A:133:ARG:H	1.36	0.73
1:B:40:ARG:CD	1:B:378:THR:O	2.37	0.73
1:C:195:GLY:H	1:C:199:ASN:HD22	1.37	0.72
1:C:78:GLN:HE22	1:C:133:ARG:H	1.39	0.71
1:A:243:ARG:HD3	1:A:286:ASP:CG	2.10	0.71
1:C:375:TYR:CZ	2:C:501:FMN:HM72	2.27	0.70
1:A:195:GLY:H	1:A:199:ASN:HD22	1.40	0.70
1:C:25:ASN:HD21	1:C:186:ASP:HB3	1.55	0.70
1:B:130:GLU:OE1	3:B:858:HOH:O	2.10	0.69
1:A:235:VAL:O	1:A:239:ARG:HD3	1.93	0.68
1:A:29:HIS:HD2	1:A:31:VAL:H	1.42	0.67
1:A:133:ARG:HD3	1:A:159:HIS:CD2	2.29	0.67
1:B:40:ARG:HD3	1:B:378:THR:O	1.94	0.66
1:A:353:ASN:HD21	1:A:367:ASN:N	1.91	0.65
1:D:78:GLN:HE22	1:D:133:ARG:H	1.45	0.65
1:D:195:GLY:H	1:D:199:ASN:HD22	1.43	0.65
1:D:235:VAL:O	1:D:239:ARG:HD3	1.97	0.63
1:C:40:ARG:O	1:C:49:ASN:HB2	1.99	0.63
1:B:375:TYR:CZ	2:B:501:FMN:HM72	2.36	0.61
1:B:375:TYR:CE1	2:B:501:FMN:HM72	2.38	0.59
1:D:7:ASP:OD1	1:D:398:LYS:NZ	2.32	0.58
1:B:195:GLY:H	1:B:199:ASN:HD22	1.48	0.58
1:D:390:GLU:OE1	3:D:601:HOH:O	2.17	0.58
1:D:14:THR:CG2	1:D:16:ILE:H	2.15	0.58
1:A:243:ARG:CD	1:A:286:ASP:CG	2.73	0.57
1:C:167:LYS:HE3	1:C:167:LYS:O	2.05	0.57
1:B:371:ARG:HD2	3:B:744:HOH:O	2.05	0.56
1:D:11:LEU:O	1:D:14:THR:HB	2.06	0.55
1:C:105:HIS:HE1	1:C:186:ASP:OD2	1.90	0.55
1:B:243:ARG:HD2	1:B:286:ASP:CG	2.28	0.54
1:B:235:VAL:O	1:B:239:ARG:HD2	2.08	0.54
1:C:120:ARG:HD2	1:C:200:GLN:HG2	1.90	0.53
1:C:195:GLY:H	1:C:199:ASN:ND2	2.04	0.53
1:A:243:ARG:HD2	1:A:286:ASP:OD1	2.07	0.53
1:C:29:HIS:HD2	1:C:31:VAL:H	1.57	0.53
1:A:243:ARG:HD3	1:A:286:ASP:OD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ARG:HH21	2:B:501:FMN:C2	2.22	0.53
1:C:261:ILE:HD12	3:C:636:HOH:O	2.10	0.52
1:D:14:THR:HG23	1:D:16:ILE:H	1.74	0.52
1:D:195:GLY:H	1:D:199:ASN:ND2	2.08	0.52
1:A:129:LYS:HD3	1:A:129:LYS:N	2.25	0.51
1:B:171:LYS:HB3	1:B:171:LYS:NZ	2.25	0.51
1:B:195:GLY:H	1:B:199:ASN:ND2	2.08	0.51
1:C:243:ARG:NH2	2:C:501:FMN:N1	2.59	0.51
1:A:375:TYR:CZ	2:A:501:FMN:HM72	2.47	0.50
1:D:25:ASN:HD21	1:D:186:ASP:HB3	1.77	0.50
1:B:235:VAL:O	1:B:239:ARG:CD	2.61	0.48
1:D:289:GLU:OE2	1:D:322:ARG:HD2	2.14	0.48
1:C:67:LEU:HD11	1:C:112:TRP:CD1	2.49	0.48
1:C:91:LYS:HA	1:C:91:LYS:HE3	1.95	0.48
1:D:289:GLU:OE2	1:D:322:ARG:CD	2.61	0.48
1:B:25:ASN:HD21	1:B:186:ASP:HB3	1.78	0.48
1:B:371:ARG:HD3	1:B:374:PHE:CE2	2.50	0.47
1:B:40:ARG:O	1:B:49:ASN:HB2	2.15	0.47
1:B:164:GLU:HG3	3:B:856:HOH:O	2.15	0.47
1:C:222:ARG:HG3	3:C:718:HOH:O	2.14	0.46
1:D:9:LYS:HE3	1:D:331:ASP:OD1	2.16	0.46
1:A:348:ARG:NH1	2:A:501:FMN:O3P	2.49	0.46
1:A:195:GLY:H	1:A:199:ASN:ND2	2.10	0.45
1:A:235:VAL:O	1:A:239:ARG:CD	2.63	0.45
1:A:25:ASN:HD21	1:A:186:ASP:HB3	1.82	0.45
1:A:40:ARG:O	1:A:49:ASN:HB2	2.16	0.44
1:A:37:THR:O	2:A:501:FMN:H6	2.17	0.44
1:D:221:ALA:HB1	1:D:268:VAL:HG22	1.99	0.44
2:C:501:FMN:H1'1	3:C:763:HOH:O	2.17	0.43
1:A:142:TYR:CD1	1:A:148:LYS:HA	2.53	0.43
1:D:375:TYR:CZ	2:D:501:FMN:HM72	2.54	0.43
1:A:167:LYS:HG2	3:A:632:HOH:O	2.18	0.43
1:A:39:MET:HA	1:A:84:ASN:O	2.19	0.42
1:A:29:HIS:CD2	1:A:31:VAL:H	2.30	0.42
1:C:92:GLU:CD	3:C:752:HOH:O	2.58	0.42
1:C:133:ARG:NH2	3:C:725:HOH:O	2.42	0.41
1:B:243:ARG:HD2	1:B:286:ASP:OD2	2.20	0.41
1:B:243:ARG:NH2	2:B:501:FMN:N1	2.60	0.41
1:D:14:THR:HG22	1:D:16:ILE:H	1.83	0.41
1:C:67:LEU:CD1	1:C:112:TRP:CD1	3.03	0.41
1:A:177:ALA:O	1:A:181:ILE:HG12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:TYR:CD1	1:D:148:LYS:HA	2.55	0.41
1:C:4:MET:CE	3:C:659:HOH:O	2.67	0.41
1:B:40:ARG:HD2	1:B:378:THR:O	2.19	0.41
1:C:4:MET:HE3	1:C:366:LEU:HD12	2.03	0.41
1:B:221:ALA:HB1	1:B:268:VAL:HG22	2.02	0.41
1:A:310:GLU:OE1	1:A:339:LYS:HE2	2.21	0.40
1:D:105:HIS:HE1	1:D:184:GLY:O	2.03	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	388/403 (96%)	379 (98%)	9 (2%)	0	100	100
1	B	370/403 (92%)	358 (97%)	12 (3%)	0	100	100
1	C	377/403 (94%)	366 (97%)	11 (3%)	0	100	100
1	D	379/403 (94%)	370 (98%)	9 (2%)	0	100	100
All	All	1514/1612 (94%)	1473 (97%)	41 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	329/340 (97%)	320 (97%)	9 (3%)	52	36
1	B	313/340 (92%)	307 (98%)	6 (2%)	65	52
1	C	318/340 (94%)	308 (97%)	10 (3%)	47	30
1	D	320/340 (94%)	314 (98%)	6 (2%)	65	52
All	All	1280/1360 (94%)	1249 (98%)	31 (2%)	57	41

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PHE
1	A	27	LEU
1	A	129	LYS
1	A	167	LYS
1	A	182	ASP
1	A	239	ARG
1	A	243	ARG
1	A	328	LEU
1	A	350	PHE
1	B	94	LEU
1	B	218	GLU
1	B	243	ARG
1	B	310	GLU
1	B	350	PHE
1	B	371	ARG
1	C	6	PHE
1	C	91	LYS
1	C	120	ARG
1	C	141	LEU
1	C	156	ASN
1	C	171	LYS
1	C	328	LEU
1	C	335	LEU
1	C	350	PHE
1	C	389	GLU
1	D	1	MET
1	D	14	THR
1	D	156	ASN
1	D	191	HIS
1	D	223	PHE
1	D	350	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	29	HIS
1	A	78	GLN
1	A	84	ASN
1	A	107	ASN
1	A	199	ASN
1	A	353	ASN
1	B	25	ASN
1	B	62	GLN
1	B	107	ASN
1	B	199	ASN
1	B	309	ASN
1	B	372	ASN
1	C	25	ASN
1	C	29	HIS
1	C	78	GLN
1	C	84	ASN
1	C	156	ASN
1	C	199	ASN
1	C	309	ASN
1	C	341	ASN
1	D	5	ASN
1	D	24	ASN
1	D	25	ASN
1	D	62	GLN
1	D	78	GLN
1	D	107	ASN
1	D	156	ASN
1	D	199	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	11 (34%)	34,50,50	2.91	6 (17%)
2	FMN	B	501	-	32,33,33	2.21	9 (28%)	34,50,50	2.51	12 (35%)
2	FMN	C	501	-	32,33,33	2.26	11 (34%)	34,50,50	2.58	9 (26%)
2	FMN	D	501	-	32,33,33	1.72	8 (25%)	34,50,50	2.52	9 (26%)

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
2	FMN	B	501	-	-	0/18/18/18	0/3/3/3
2	FMN	C	501	-	-	0/18/18/18	0/3/3/3
2	FMN	D	501	-	-	0/18/18/18	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FMN	C2-N1	-3.00	1.31	1.38
2	C	501	FMN	C1'-N10	-2.38	1.45	1.48
2	B	501	FMN	C9A-N10	2.03	1.41	1.38
2	D	501	FMN	C9A-C5A	2.08	1.47	1.42
2	A	501	FMN	O4-C4	2.10	1.29	1.24
2	C	501	FMN	P-O5'	2.11	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FMN	O4-C4	2.12	1.30	1.24
2	D	501	FMN	C4-N3	2.22	1.37	1.33
2	A	501	FMN	P-O5'	2.23	1.66	1.59
2	B	501	FMN	O3'-C3'	2.25	1.48	1.43
2	D	501	FMN	C8-C7	2.29	1.47	1.41
2	C	501	FMN	C4A-N5	2.39	1.37	1.33
2	A	501	FMN	C9A-C5A	2.51	1.47	1.42
2	A	501	FMN	C4-N3	2.52	1.37	1.33
2	A	501	FMN	C4-C4A	2.53	1.46	1.41
2	A	501	FMN	O3'-C3'	2.54	1.48	1.43
2	C	501	FMN	O4-C4	2.55	1.31	1.24
2	B	501	FMN	C4-N3	2.70	1.37	1.33
2	C	501	FMN	O3'-C3'	2.85	1.49	1.43
2	C	501	FMN	C4-N3	2.90	1.38	1.33
2	C	501	FMN	C9A-C5A	2.98	1.48	1.42
2	C	501	FMN	C9A-N10	3.08	1.43	1.38
2	A	501	FMN	C4A-N5	3.10	1.38	1.33
2	D	501	FMN	O3'-C3'	3.29	1.50	1.43
2	D	501	FMN	C4A-C10	3.30	1.46	1.40
2	A	501	FMN	C8-C7	3.34	1.50	1.41
2	D	501	FMN	C4A-N5	3.43	1.38	1.33
2	B	501	FMN	O4-C4	3.45	1.33	1.24
2	C	501	FMN	C8-C7	3.46	1.50	1.41
2	B	501	FMN	C4A-N5	3.49	1.38	1.33
2	B	501	FMN	C9A-C5A	3.57	1.50	1.42
2	D	501	FMN	C4-C4A	3.62	1.48	1.41
2	B	501	FMN	C8-C7	4.27	1.52	1.41
2	A	501	FMN	C4A-C10	4.83	1.49	1.40
2	A	501	FMN	C9A-N10	4.86	1.45	1.38
2	B	501	FMN	C4-C4A	5.25	1.52	1.41
2	C	501	FMN	C4A-C10	5.30	1.50	1.40
2	B	501	FMN	C4A-C10	6.28	1.52	1.40
2	C	501	FMN	C4-C4A	6.58	1.54	1.41

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	FMN	C4A-C4-N3	-6.51	115.02	123.52
2	B	501	FMN	C4A-C4-N3	-6.19	115.43	123.52
2	C	501	FMN	C4A-C4-N3	-5.30	116.60	123.52
2	D	501	FMN	C4A-C4-N3	-4.98	117.01	123.52
2	D	501	FMN	C4-C4A-C10	-4.08	117.33	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	FMN	C4-C4A-C10	-3.83	117.49	119.94
2	D	501	FMN	N3-C2-N1	-3.23	122.25	127.69
2	C	501	FMN	O3P-P-O5'	-2.90	98.26	106.72
2	A	501	FMN	N3-C2-N1	-2.84	122.92	127.69
2	B	501	FMN	O2'-C2'-C3'	-2.74	101.90	108.96
2	B	501	FMN	C4-C4A-C10	-2.59	118.29	119.94
2	B	501	FMN	O5'-P-O1P	-2.58	100.60	107.08
2	C	501	FMN	C4-C4A-C10	-2.49	118.35	119.94
2	B	501	FMN	O3'-C3'-C4'	2.18	114.37	108.73
2	C	501	FMN	O3P-P-O2P	2.20	115.52	107.44
2	B	501	FMN	O3P-P-O1P	2.37	118.36	110.63
2	C	501	FMN	O2'-C2'-C1'	2.51	116.13	109.93
2	B	501	FMN	C4-C4A-N5	2.58	121.84	118.70
2	B	501	FMN	O2'-C2'-C1'	2.61	116.39	109.93
2	D	501	FMN	C6-C5A-C9A	2.84	122.24	119.11
2	D	501	FMN	O3'-C3'-C4'	2.85	116.12	108.73
2	B	501	FMN	C1'-N10-C9A	2.87	122.16	118.83
2	D	501	FMN	C4-C4A-N5	3.07	122.43	118.70
2	B	501	FMN	C4A-N5-C5A	3.56	120.92	116.72
2	D	501	FMN	C5A-C9A-N10	3.60	120.28	117.58
2	D	501	FMN	C4A-N5-C5A	3.81	121.22	116.72
2	C	501	FMN	O3'-C3'-C4'	3.97	119.02	108.73
2	B	501	FMN	C5A-C9A-N10	4.00	120.58	117.58
2	A	501	FMN	C4-C4A-N5	4.27	123.89	118.70
2	C	501	FMN	C4-C4A-N5	5.76	125.70	118.70
2	A	501	FMN	C4A-N5-C5A	6.12	123.93	116.72
2	C	501	FMN	C4-N3-C2	6.32	120.43	115.16
2	C	501	FMN	C4A-N5-C5A	7.52	125.59	116.72
2	B	501	FMN	C4-N3-C2	8.59	122.33	115.16
2	D	501	FMN	C4-N3-C2	9.13	122.78	115.16
2	A	501	FMN	C4-N3-C2	11.91	125.10	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FMN	3	0
2	B	501	FMN	4	0
2	C	501	FMN	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	FMN	1	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	390/403 (96%)	-0.23	9 (2%) 64 59	12, 17, 34, 56	0
1	B	374/403 (92%)	-0.49	1 (0%) 94 92	9, 14, 24, 40	0
1	C	381/403 (94%)	-0.08	10 (2%) 59 54	12, 23, 36, 47	0
1	D	383/403 (95%)	2.04	175 (45%) 0 0	27, 43, 71, 90	0
All	All	1528/1612 (94%)	0.31	195 (12%) 5 4	9, 21, 56, 90	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	134	TYR	8.0
1	D	85	VAL	7.0
1	D	151	ALA	6.4
1	D	202	LEU	6.2
1	D	197	LEU	6.0
1	D	41	ALA	5.6
1	D	48	PRO	5.6
1	D	74	PHE	5.5
1	D	382	TYR	5.5
1	D	198	LEU	5.5
1	D	88	ILE	5.3
1	D	86	PRO	5.2
1	D	127	LEU	5.2
1	D	89	TRP	5.1
1	A	293	THR	5.0
1	D	351	ILE	4.9
1	D	79	SER	4.8
1	D	195	GLY	4.8
1	D	118	LEU	4.8
1	D	346	TYR	4.7
1	D	262	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	161	ILE	4.6
1	D	137	ALA	4.6
1	D	221	ALA	4.6
1	D	366	LEU	4.6
1	D	201	PHE	4.5
1	D	119	GLY	4.5
1	D	352	ALA	4.5
1	D	81	GLY	4.5
1	D	144	GLY	4.5
1	D	213	TYR	4.5
1	D	158	GLN	4.4
1	D	244	PHE	4.4
1	D	193	ALA	4.4
1	A	292	VAL	4.4
1	D	378	THR	4.4
1	D	117	VAL	4.4
1	D	53	ALA	4.3
1	D	360	LEU	4.3
1	D	36	LEU	4.2
1	D	135	ASP	4.2
1	D	381	GLY	4.0
1	D	385	TYR	4.0
1	D	32	VAL	3.9
1	D	100	ILE	3.9
1	D	376	THR	3.9
1	D	196	TYR	3.9
1	D	38	ARG	3.9
1	D	350	PHE	3.8
1	D	323	VAL	3.8
1	D	122	ALA	3.8
1	D	265	TYR	3.8
1	D	31	VAL	3.8
1	D	269	ILE	3.8
1	D	87	GLY	3.7
1	D	253	MET	3.7
1	D	200	GLN	3.7
1	D	224	THR	3.7
1	D	356	LEU	3.7
1	D	126	VAL	3.7
1	D	111	VAL	3.6
1	D	169	TYR	3.6
1	D	396	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	84	ASN	3.6
1	D	45	GLY	3.6
1	D	47	ILE	3.6
1	D	97	TRP	3.6
1	D	80	GLY	3.6
1	D	156	ASN	3.5
1	D	136	SER	3.5
1	D	242	ILE	3.5
1	A	300	PHE	3.5
1	D	357	VAL	3.5
1	D	138	THR	3.5
1	D	68	ILE	3.4
1	C	393	ALA	3.4
1	D	46	ASN	3.3
1	D	73	THR	3.3
1	D	377	PHE	3.3
1	D	205	ILE	3.3
1	D	124	PRO	3.3
1	D	207	ASN	3.2
1	D	37	THR	3.2
1	D	203	ASP	3.2
1	D	288	VAL	3.2
1	A	297	LEU	3.2
1	D	223	PHE	3.2
1	D	285	ILE	3.2
1	D	159	HIS	3.1
1	D	373	THR	3.1
1	D	166	ILE	3.1
1	D	375	TYR	3.1
1	D	77	ALA	3.1
1	D	349	SER	3.1
1	D	42	ILE	3.1
1	D	245	SER	3.0
1	D	287	LEU	3.0
1	D	39	MET	3.0
1	D	344	ILE	3.0
1	D	374	PHE	3.0
1	D	57	TYR	3.0
1	D	76	SER	3.0
1	D	386	PRO	3.0
1	D	372	ASN	3.0
1	D	268	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	248	GLY	2.9
1	C	7	ASP	2.9
1	D	380	GLU	2.9
1	D	113	VAL	2.8
1	C	1	MET	2.8
1	D	160	GLY	2.8
1	D	247	TYR	2.8
1	A	294	ASP	2.8
1	D	70	THR	2.8
1	D	264	GLN	2.8
1	D	132	LEU	2.8
1	D	327	ALA	2.8
1	D	272	LEU	2.8
1	D	354	PRO	2.8
1	D	143	MET	2.8
1	D	72	GLY	2.7
1	D	199	ASN	2.7
1	D	206	SER	2.7
1	D	217	ILE	2.7
1	D	353	ASN	2.7
1	D	11	LEU	2.7
1	D	282	LEU	2.7
1	D	155	ASN	2.7
1	D	176	ALA	2.7
1	D	384	ASP	2.7
1	D	16	ILE	2.6
1	A	392	VAL	2.6
1	D	56	TYR	2.6
1	D	324	GLY	2.6
1	D	261	ILE	2.6
1	D	383	THR	2.6
1	D	112	TRP	2.6
1	D	392	VAL	2.6
1	D	133	ARG	2.6
1	D	228	VAL	2.6
1	D	120	ARG	2.5
1	D	393	ALA	2.5
1	D	52	TRP	2.5
1	D	78	GLN	2.5
1	D	94	LEU	2.5
1	D	347	GLY	2.5
1	D	157	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	40	ARG	2.5
1	D	141	LEU	2.5
1	D	246	PRO	2.4
1	D	104	ILE	2.4
1	D	33	MET	2.4
1	D	142	TYR	2.4
1	D	115	LEU	2.4
1	D	152	LEU	2.4
1	D	343	LEU	2.4
1	D	116	TRP	2.4
1	D	173	TYR	2.3
1	D	345	GLY	2.3
1	D	367	ASN	2.3
1	D	101	PHE	2.3
1	D	35	ALA	2.3
1	D	220	ARG	2.2
1	D	225	LEU	2.2
1	A	5	ASN	2.2
1	D	50	THR	2.2
1	D	83	PRO	2.2
1	D	284	PHE	2.2
1	D	71	GLU	2.2
1	D	121	GLN	2.2
1	D	190	ILE	2.2
1	D	326	TYR	2.2
1	B	257	GLU	2.2
1	D	321	LEU	2.2
1	C	210	THR	2.2
1	C	279	GLY	2.2
1	D	263	ALA	2.2
1	C	394	LYS	2.1
1	D	147	GLU	2.1
1	D	257	GLU	2.1
1	C	5	ASN	2.1
1	C	397	LYS	2.1
1	A	3	TYR	2.1
1	D	359	ARG	2.1
1	C	234	ALA	2.1
1	D	260	GLY	2.1
1	D	307	GLY	2.1
1	D	75	PRO	2.1
1	D	67	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	277	ARG	2.0
1	D	93	GLN	2.0
1	D	154	ALA	2.0
1	D	312	ILE	2.0
1	D	387	SER	2.0
1	A	391	SER	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 (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. 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
2	FMN	C	501	31/31	0.86	0.23	6.07	20,27,32,33	0
2	FMN	B	501	31/31	0.91	0.18	3.88	14,18,22,24	0
2	FMN	A	501	31/31	0.91	0.15	2.84	15,20,23,24	0
2	FMN	D	501	31/31	0.93	0.13	-2.36	17,19,22,23	0

6.5 Other polymers (i)

There are no such residues in this entry.