wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 06:55 PM GMT

PDB ID	:	1D4C
Title	:	CRYSTAL STRUCTURE OF THE UNCOMPLEXED FORM OF THE FLAVOCYTOCHROME C FUMARATE REDUCTASE OF SHEWANELLA PUTREFACIENS STRAIN MR-1
Authors	:	Leys, D.; Tsapin, A.S.; Meyer, T.E.; Cusanovich, M.A.; Van Beeumen, J.J.
Deposited on	:	1999-10-03
Resolution	:	2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i)) were used in the production of this report:

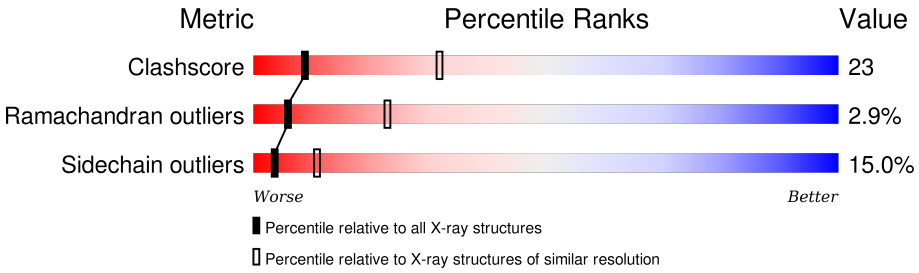
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	572	51% 35% 12% •
1	B	572	51% 35% 11% ••
1	C	572	51% 33% 13% ••
1	D	572	50% 37% 12% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FAD	A	600	X	-	-	-
4	FAD	B	700	X	-	-	-
4	FAD	C	800	X	-	-	-
4	FAD	D	900	X	-	-	-

2 Entry composition (i)

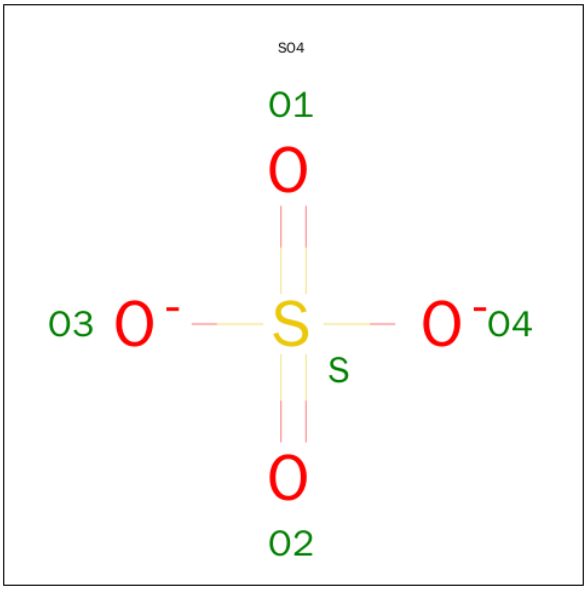
There are 5 unique types of molecules in this entry. The entry contains 17470 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FLAVOCYTOCHROME C FUMARATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	570	Total	C	N	O	S	0	0	0
			4124	2562	736	807	19			
1	B	566	Total	C	N	O	S	0	0	0
			4093	2542	731	801	19			
1	C	568	Total	C	N	O	S	0	0	0
			4099	2546	733	801	19			
1	D	570	Total	C	N	O	S	0	0	0
			4113	2553	734	807	19			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



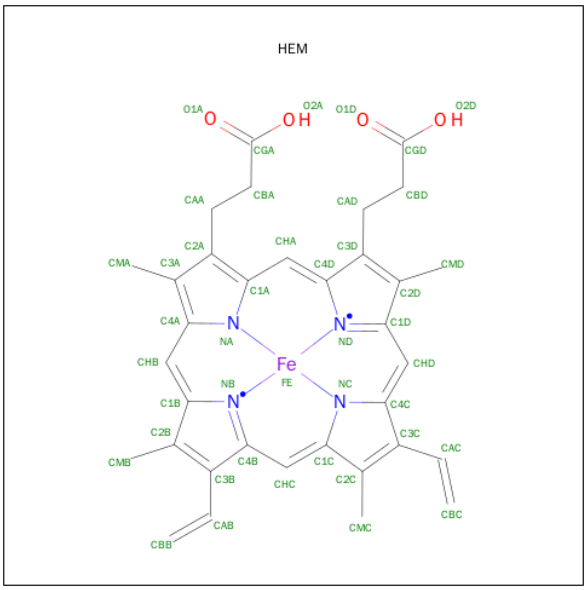
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



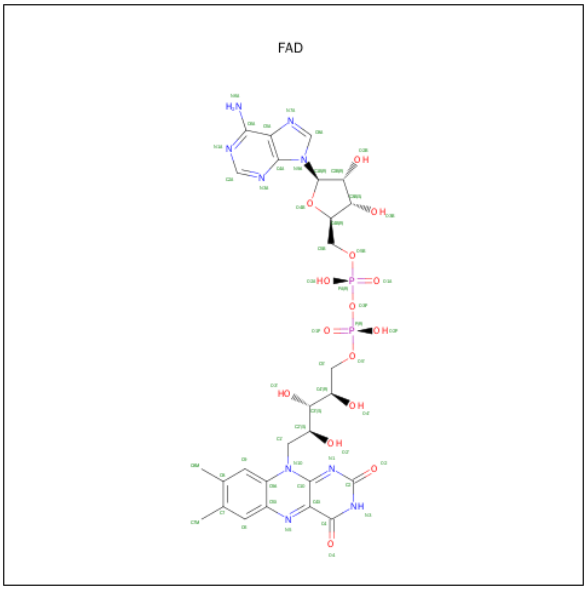
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Fe N O 43 34 1 4 4	0	0
3	A	1	Total C Fe N O 43 34 1 4 4	0	0
3	A	1	Total C Fe N O 43 34 1 4 4	0	0
3	A	1	Total C Fe N O 43 34 1 4 4	0	0
3	B	1	Total C Fe N O 43 34 1 4 4	0	0
3	B	1	Total C Fe N O 43 34 1 4 4	0	0
3	B	1	Total C Fe N O 43 34 1 4 4	0	0
3	B	1	Total C Fe N O 43 34 1 4 4	0	0
3	C	1	Total C Fe N O 43 34 1 4 4	0	0
3	C	1	Total C Fe N O 43 34 1 4 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	48	Total O 48 48	0	0
5	B	29	Total O 29 29	0	0
5	C	30	Total O 30 30	0	0
5	D	19	Total O 19 19	0	0

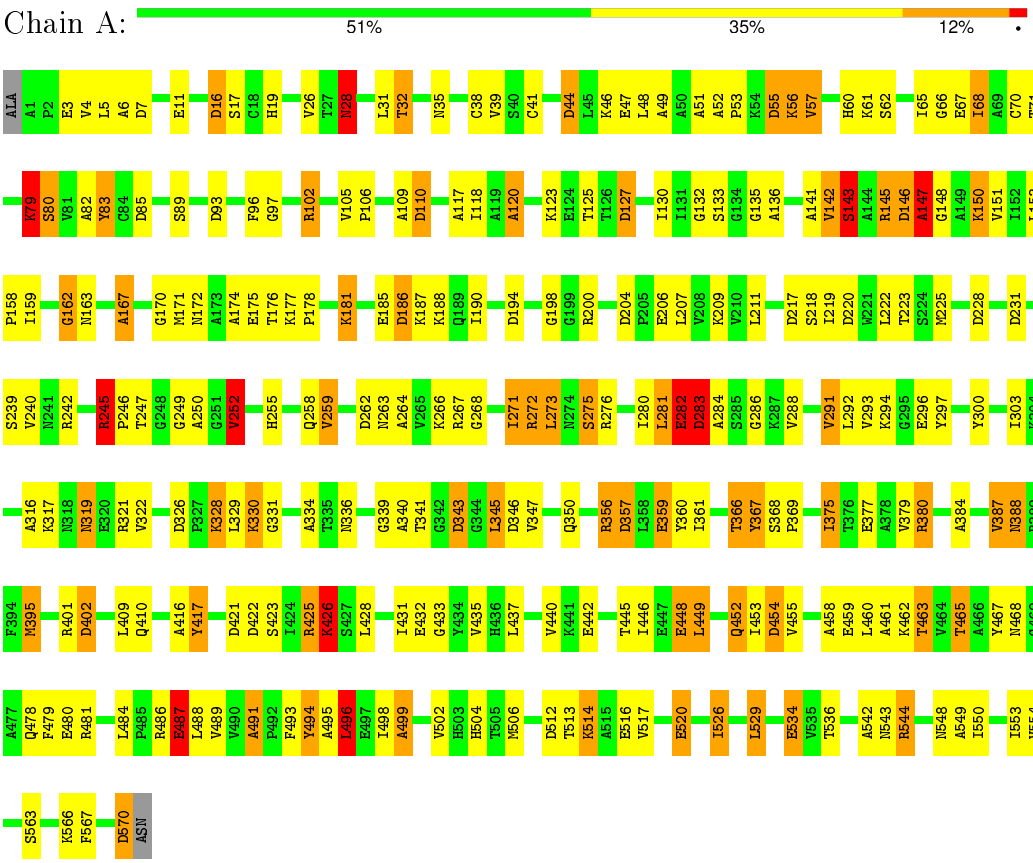
3 Residue-property plots (i)

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.

Note EDS was not executed.

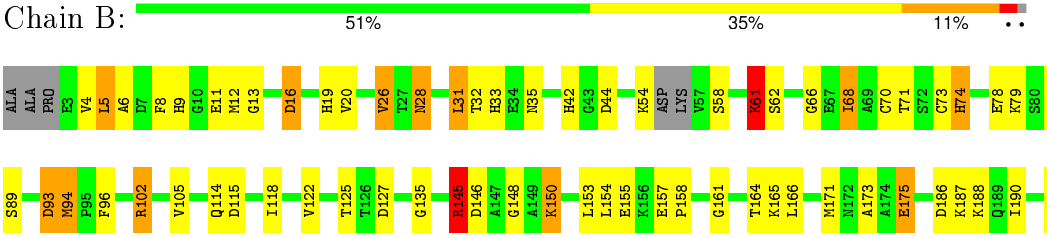
• Molecule 1: FLAVOCYTOCHROME C FUMARATE REDUCTASE

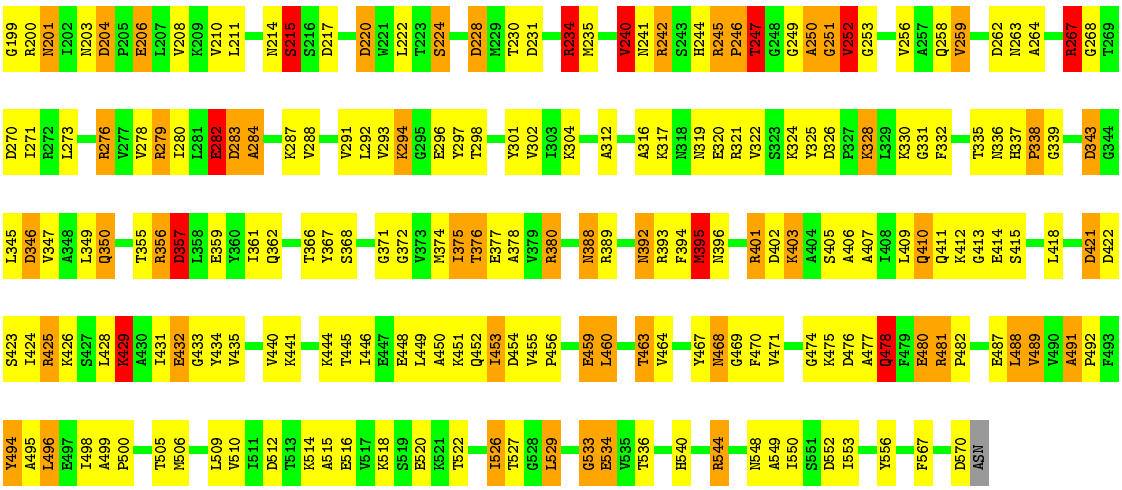
Chain A:



• Molecule 1: FLAVOCYTOCHROME C FUMARATE REDUCTASE

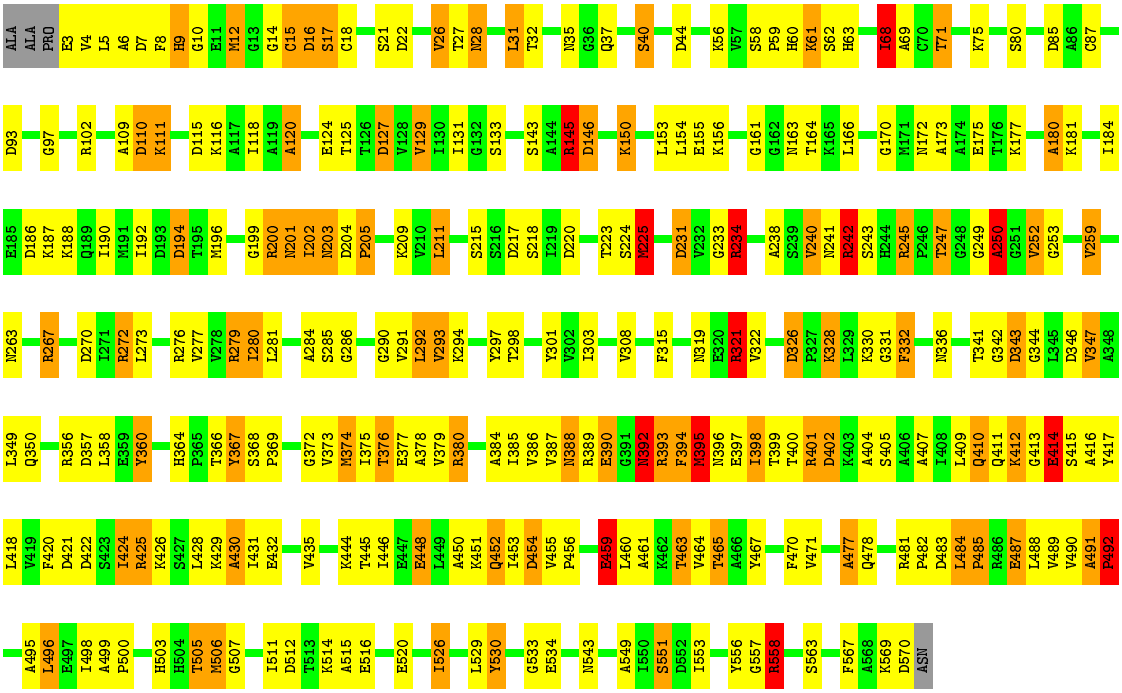
Chain B:





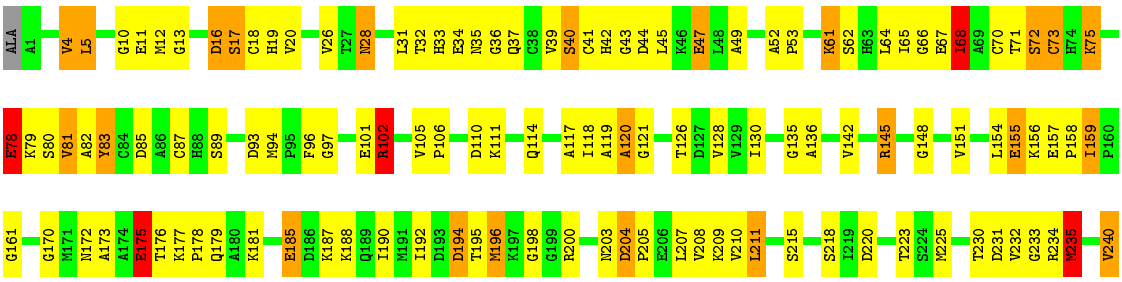
• Molecule 1: FLAVOCYTOCHROME C FUMARATE REDUCTASE

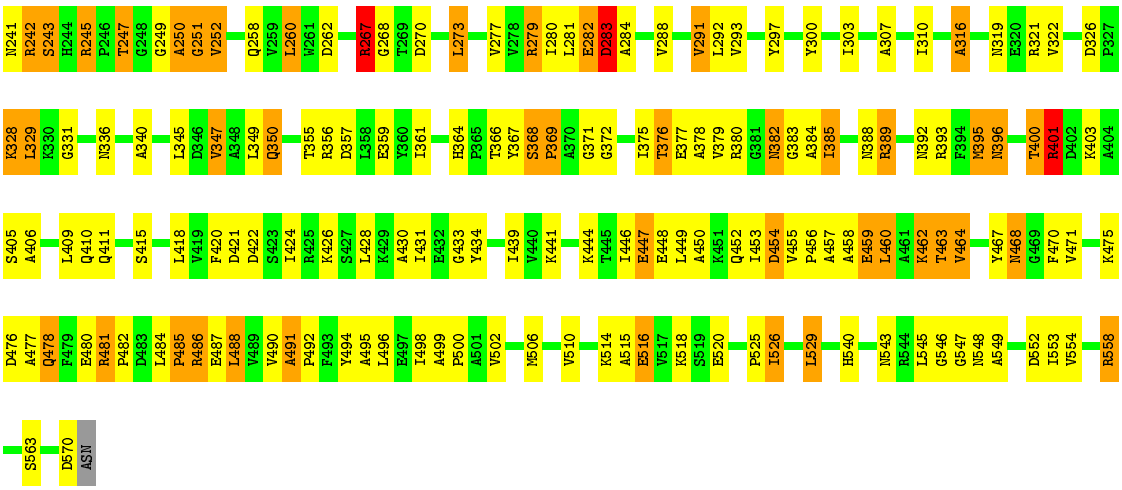
Chain C:



• Molecule 1: FLAVOCYTOCHROME C FUMARATE REDUCTASE

Chain D:




N241 R242 S243 H244 R245 P246 T247 G248 G249 A250 G251 V252 Q258 Y259 L260 W261 D262 R267 G268 T269 D270 L273 V277 V278 R279 I280 L281 E282 D283 A284 V288 V291 L292 V293 Y297 Y300 I303 A307 I310 A316 N319 E320 R321 V322 D326 P327
K328 L329 K330 G331 N336 A340 L345 D346 V347 A348 L349 Q350 T355 R356 D357 L358 E359 Y360 I361 H364 P365 T366 Y367 S368 P369 A370 G371 G372 I375 T376 E377 A378 V379 R380 G381 N382 G383 A384 I385 N388 R389 N392 R393 F394 M395 N396 T400 R401 D402 K403 A404
S405 A406 L409 Q410 Q411 S415 L418 V419 F420 D421 D422 S423 I424 R425 K426 S427 L428 K429 A430 I431 E432 G433 Y434 I439 V440 K441 K444 T445 I446 E447 F448 L449 A450 K451 Q452 I453 D454 V455 P456 A457 A458 E459 L460 A461 K462 T463 V464 Y467 N468 G469 F470 V471 K475
D476 A477 Q478 F479 E480 R481 P482 D483 L484 P485 R486 E487 I488 V489 V490 A491 P492 F493 Y494 A495 L496 E497 I498 A499 P500 A501 V502 M506 V510 K514 A515 E516 V517 K518 S519 E520 P525 I526 L529 H540 N543 R544 I545 G546 G547 N548 A549 D552 I553 V554 R558
S563 D570 ASN

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	109.69Å 216.36Å 112.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90	Depositor
% Data completeness (in resolution range)	93.7 (15.00-2.90)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.210 , 0.300	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17470	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.76	0/4192	2.22	144/5683 (2.5%)
1	B	0.74	7/4159 (0.2%)	1.97	112/5637 (2.0%)
1	C	0.71	3/4166 (0.1%)	2.04	126/5649 (2.2%)
1	D	0.64	1/4179 (0.0%)	1.94	98/5665 (1.7%)
All	All	0.72	11/16696 (0.1%)	2.05	480/22634 (2.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	3
1	D	0	2
All	All	0	10

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	480	GLU	CD-OE1	9.81	1.36	1.25
1	C	459	GLU	CD-OE1	9.29	1.35	1.25
1	C	459	GLU	CD-OE2	8.55	1.35	1.25
1	B	476	ASP	CG-OD1	8.47	1.44	1.25
1	B	459	GLU	CD-OE2	7.25	1.33	1.25

The worst 5 of 480 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	245	ARG	CD-NE-CZ	29.02	164.23	123.60
1	A	267	ARG	CD-NE-CZ	24.00	157.20	123.60
1	A	102	ARG	NE-CZ-NH2	23.33	131.97	120.30
1	D	401	ARG	CD-NE-CZ	21.85	154.19	123.60
1	D	242	ARG	NE-CZ-NH1	20.69	130.65	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	ASP	Mainchain
1	A	491	ALA	Mainchain,Peptide
1	B	491	ALA	Mainchain,Peptide
1	C	477	ALA	Mainchain
1	C	491	ALA	Mainchain

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	4124	0	4013	181	1
1	B	4093	0	3976	179	0
1	C	4099	0	3977	192	2
1	D	4113	0	3987	210	1
2	B	5	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	172	0	120	15	0
3	B	172	0	120	17	0
3	C	172	0	120	13	0
3	D	172	0	120	19	0
4	A	53	0	31	9	0
4	B	53	0	31	8	0
4	C	53	0	31	12	0
4	D	53	0	30	9	0
5	A	48	0	0	2	0
5	B	29	0	0	3	0
5	C	30	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	19	0	0	2	0
All	All	17470	0	16556	789	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 23.

The worst 5 of 789 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:D:70:CYS:SG	3:D:602:HEM:HAB	1.27	1.72
1:D:18:CYS:SG	3:D:603:HEM:HAC	1.21	1.71
1:D:41:CYS:SG	3:D:604:HEM:HAC	1.13	1.70
1:B:87:CYS:SG	3:B:601:HEM:HAC	1.33	1.68
4:B:700:FAD:C2'	4:B:700:FAD:C1'	1.77	1.62

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)
1:A:125:THR:OG1	1:C:247:THR:OG1[4_555]	2.12	0.08
1:C:125:THR:OG1	1:D:247:THR:OG1[4_456]	2.15	0.05

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	568/572 (99%)	504 (89%)	51 (9%)	13 (2%)	8 30
1	B	562/572 (98%)	495 (88%)	52 (9%)	15 (3%)	6 25
1	C	566/572 (99%)	482 (85%)	64 (11%)	20 (4%)	4 18
1	D	566/572 (99%)	488 (86%)	61 (11%)	17 (3%)	5 22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2262/2288 (99%)	1969 (87%)	228 (10%)	65 (3%)	6 23

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	VAL
1	A	142	VAL
1	A	147	ALA
1	A	454	ASP
1	B	250	ALA

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	409/429 (95%)	350 (86%)	59 (14%)	4 12
1	B	406/429 (95%)	344 (85%)	62 (15%)	3 10
1	C	405/429 (94%)	343 (85%)	62 (15%)	3 10
1	D	407/429 (95%)	346 (85%)	61 (15%)	3 11
All	All	1627/1716 (95%)	1383 (85%)	244 (15%)	3 11

5 of 244 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	480	GLU
1	C	145	ARG
1	D	395	MET
1	B	494	TYR
1	C	17	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	410	GLN
1	C	35	ASN
1	D	388	ASN
1	B	411	GLN
1	B	478	GLN

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

23 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	$\#\|Z\| > 2$
4	FAD	A	600	-	48,58,58	1.80	11 (22%)	54,89,89	3.39	23 (42%)
3	HEM	A	601	1	30,50,50	2.63	7 (23%)	24,82,82	3.48	15 (62%)
3	HEM	A	602	1	30,50,50	2.87	9 (30%)	24,82,82	3.35	12 (50%)
3	HEM	A	603	1	30,50,50	2.71	9 (30%)	24,82,82	3.20	12 (50%)
3	HEM	A	604	1	30,50,50	2.63	10 (33%)	24,82,82	3.45	14 (58%)
3	HEM	B	601	1	30,50,50	2.66	9 (30%)	24,82,82	3.74	14 (58%)
3	HEM	B	602	1	30,50,50	2.62	8 (26%)	24,82,82	3.19	13 (54%)
3	HEM	B	603	1	30,50,50	2.65	11 (36%)	24,82,82	3.36	13 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HEM	B	604	1	30,50,50	2.71	9 (30%)	24,82,82	3.82	16 (66%)
4	FAD	B	700	-	48,58,58	1.71	8 (16%)	54,89,89	3.42	23 (42%)
2	SO4	B	714	-	4,4,4	0.65	0	6,6,6	0.65	0
3	HEM	C	601	1	30,50,50	2.72	9 (30%)	24,82,82	3.25	13 (54%)
3	HEM	C	602	1	30,50,50	3.02	10 (33%)	24,82,82	3.83	12 (50%)
3	HEM	C	603	1	30,50,50	2.54	9 (30%)	24,82,82	2.94	12 (50%)
3	HEM	C	604	1	30,50,50	2.66	8 (26%)	24,82,82	4.05	14 (58%)
4	FAD	C	800	-	48,58,58	1.58	9 (18%)	54,89,89	3.85	21 (38%)
2	SO4	C	814	-	4,4,4	0.95	0	6,6,6	0.89	1 (16%)
3	HEM	D	601	1	30,50,50	2.78	11 (36%)	24,82,82	3.39	12 (50%)
3	HEM	D	602	1	30,50,50	2.67	7 (23%)	24,82,82	3.44	12 (50%)
3	HEM	D	603	1	30,50,50	2.67	10 (33%)	24,82,82	2.89	11 (45%)
3	HEM	D	604	1	30,50,50	2.62	8 (26%)	24,82,82	3.85	18 (75%)
4	FAD	D	900	-	48,58,58	1.70	7 (14%)	54,89,89	3.57	21 (38%)
2	SO4	D	914	-	4,4,4	0.72	0	6,6,6	0.70	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
4	FAD	A	600	-	2/2/9/9	0/30/50/50	0/6/6/6
3	HEM	A	601	1	-	0/10/54/54	0/0/8/8
3	HEM	A	602	1	-	0/10/54/54	0/0/8/8
3	HEM	A	603	1	-	0/10/54/54	0/0/8/8
3	HEM	A	604	1	-	0/10/54/54	0/0/8/8
3	HEM	B	601	1	-	0/10/54/54	0/0/8/8
3	HEM	B	602	1	-	0/10/54/54	0/0/8/8
3	HEM	B	603	1	-	0/10/54/54	0/0/8/8
3	HEM	B	604	1	-	0/10/54/54	0/0/8/8
4	FAD	B	700	-	2/2/9/9	0/30/50/50	0/6/6/6
2	SO4	B	714	-	-	0/0/0/0	0/0/0/0
3	HEM	C	601	1	-	0/10/54/54	0/0/8/8
3	HEM	C	602	1	-	0/10/54/54	0/0/8/8
3	HEM	C	603	1	-	0/10/54/54	0/0/8/8
3	HEM	C	604	1	-	0/10/54/54	0/0/8/8
4	FAD	C	800	-	3/3/9/9	0/30/50/50	0/6/6/6
2	SO4	C	814	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	D	601	1	-	0/10/54/54	0/0/8/8
3	HEM	D	602	1	-	0/10/54/54	0/0/8/8
3	HEM	D	603	1	-	0/10/54/54	0/0/8/8
3	HEM	D	604	1	-	0/10/54/54	0/0/8/8
4	FAD	D	900	-	2/2/9/9	0/30/50/50	0/6/6/6
2	SO4	D	914	-	-	0/0/0/0	0/0/0/0

The worst 5 of 179 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	HEM	C3B-C4B	-11.33	1.41	1.51
3	A	602	HEM	C3B-C4B	-9.52	1.43	1.51
3	D	602	HEM	C3B-C4B	-9.26	1.43	1.51
3	B	604	HEM	C3B-C4B	-9.22	1.43	1.51
3	D	601	HEM	C3B-C4B	-9.00	1.43	1.51

The worst 5 of 302 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	604	HEM	C3B-CAB-CBB	-10.63	108.16	124.46
4	D	900	FAD	C5B-C4B-C3B	-10.38	74.02	115.21
4	A	600	FAD	C5B-C4B-C3B	-10.24	74.55	115.21
4	C	800	FAD	C5B-C4B-C3B	-10.21	74.68	115.21
4	B	700	FAD	C5B-C4B-C3B	-10.15	74.91	115.21

5 of 9 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	800	FAD	C4B
4	C	800	FAD	C4'
4	C	800	FAD	C3'
4	B	700	FAD	C4'
4	B	700	FAD	C3'

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	FAD	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	HEM	5	0
3	A	602	HEM	5	0
3	A	603	HEM	1	0
3	A	604	HEM	4	0
3	B	601	HEM	6	0
3	B	602	HEM	8	0
3	B	603	HEM	2	0
3	B	604	HEM	1	0
4	B	700	FAD	8	0
2	B	714	SO4	1	0
3	C	601	HEM	7	0
3	C	602	HEM	3	0
3	C	603	HEM	1	0
3	C	604	HEM	2	0
4	C	800	FAD	12	0
3	D	601	HEM	2	0
3	D	602	HEM	8	0
3	D	603	HEM	5	0
3	D	604	HEM	4	0
4	D	900	FAD	9	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.