



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2016 – 04:10 PM EDT

PDB ID : 3WKT
Title : Complex structure of an open form of NADPH-cytochrome P450 reductase and heme oxygenase-1
Authors : Sugishima, M.; Sato, H.; Higashimoto, Y.; Harada, J.; Wada, K.; Fukuyama, K.; Noguchi, M.
Deposited on : 2013-10-31
Resolution : 4.30 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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-20027674
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-20027674

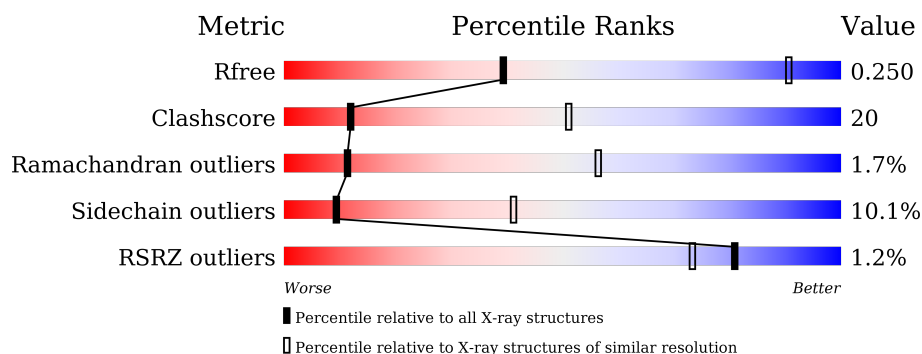
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1059 (5.00-3.60)
Clashscore	102246	1166 (5.00-3.60)
Ramachandran outliers	100387	1106 (5.00-3.60)
Sidechain outliers	100360	1089 (5.00-3.60)
RSRZ outliers	91569	1062 (5.00-3.60)

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 $\leq 5\%$. 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	618	<div> <div>%</div> <div> <div></div> <div>60%</div> <div>33%</div> <div>• •</div> </div> </div>
1	B	618	<div> <div>2%</div> <div> <div></div> <div>54%</div> <div>34%</div> <div>7%</div> <div>5%</div> </div> </div>
2	C	267	<div> <div></div> <div> <div>51%</div> <div>27%</div> <div>•</div> <div>20%</div> </div> </div>
2	D	267	<div> <div></div> <div> <div>47%</div> <div>28%</div> <div>5%</div> <div>20%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13354 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 NADPH-cytochrome P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	0	0	0
			4834	3063	830	918	23			
1	B	588	Total	C	N	O	S	0	0	0
			4720	2992	816	889	23			

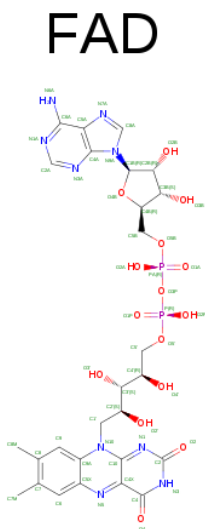
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	MET	-	EXPRESSION TAG	UNP P00388
A	?	-	THR	DELETION	UNP P00388
A	?	-	GLY	DELETION	UNP P00388
A	?	-	GLU	DELETION	UNP P00388
A	?	-	GLU	DELETION	UNP P00388
B	57	MET	-	EXPRESSION TAG	UNP P00388
B	?	-	THR	DELETION	UNP P00388
B	?	-	GLY	DELETION	UNP P00388
B	?	-	GLU	DELETION	UNP P00388
B	?	-	GLU	DELETION	UNP P00388

- Molecule 2 is a protein called Heme oxygenase 1.

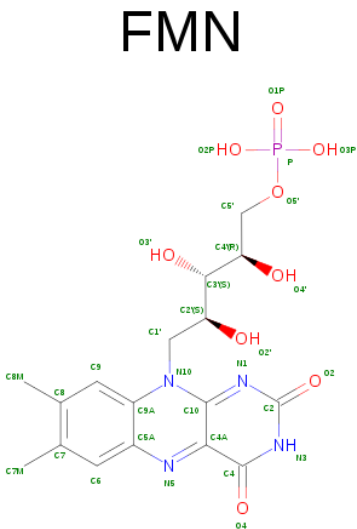
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	214	Total	C	N	O	S	0	0	0
			1742	1116	298	322	6			
2	D	214	Total	C	N	O	S	0	0	0
			1742	1116	298	322	6			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



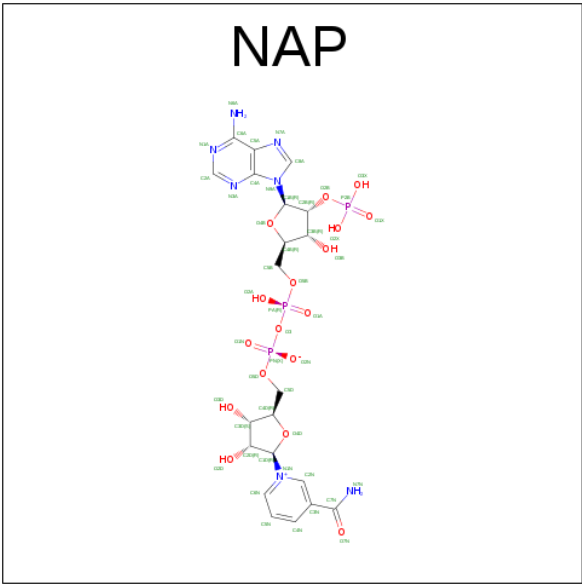
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



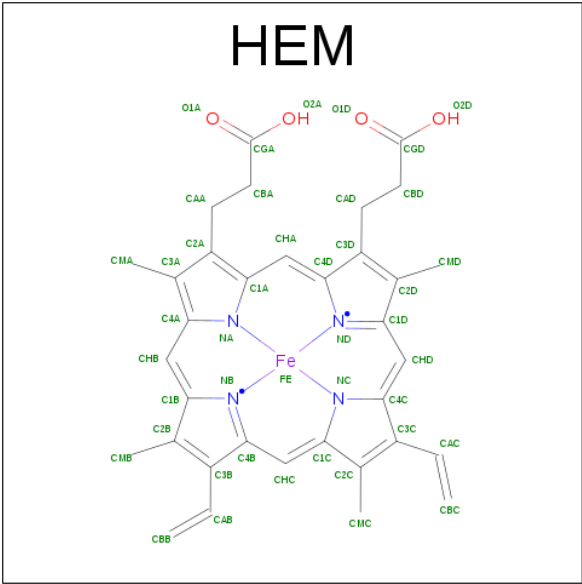
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 17	N 4	O 9	P 1	0	0
4	B	1	Total 31	C 17	N 4	O 9	P 1	0	0

- Molecule 5 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).

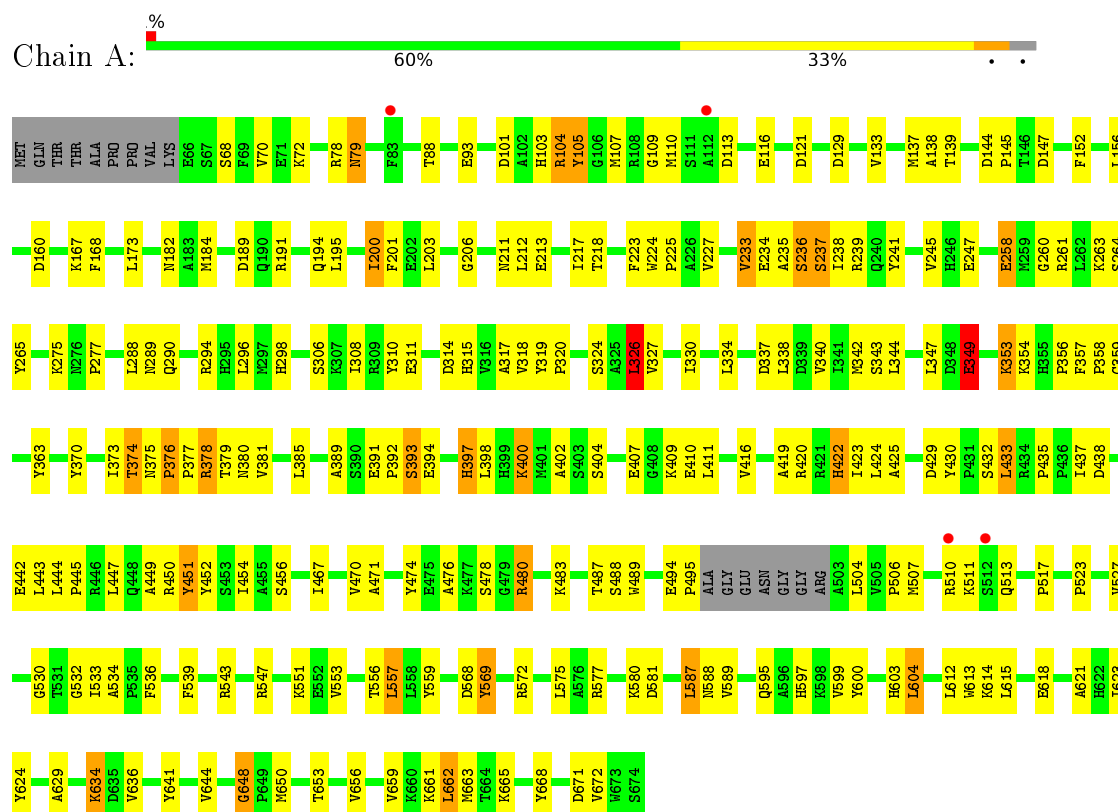


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

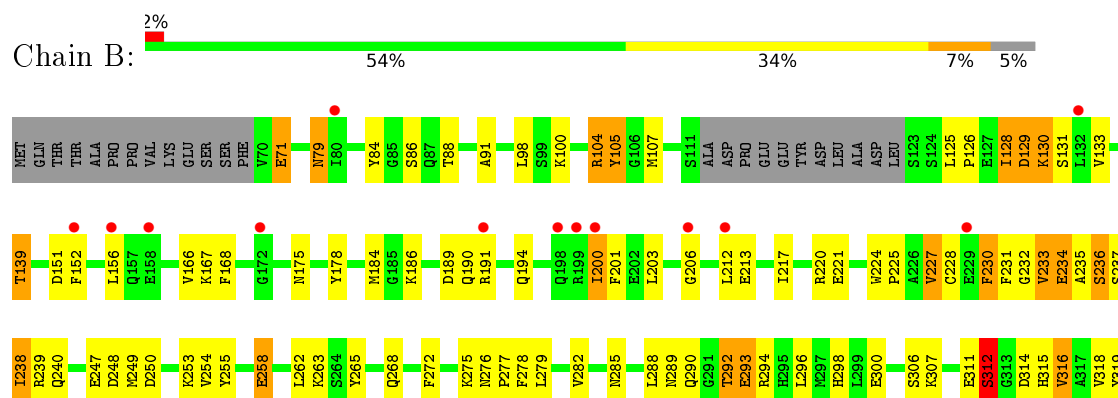
3 Residue-property plots

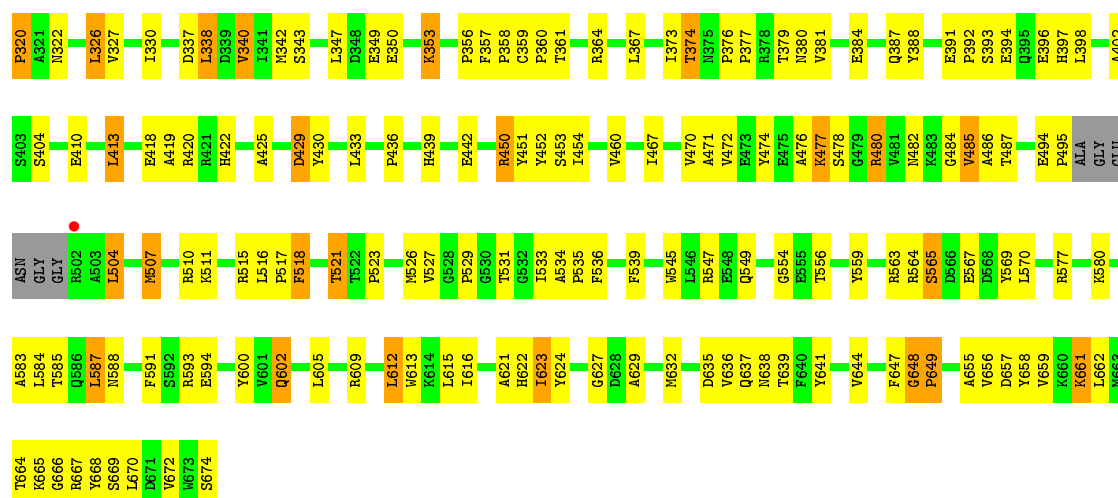
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: NADPH-cytochrome P450 reductase



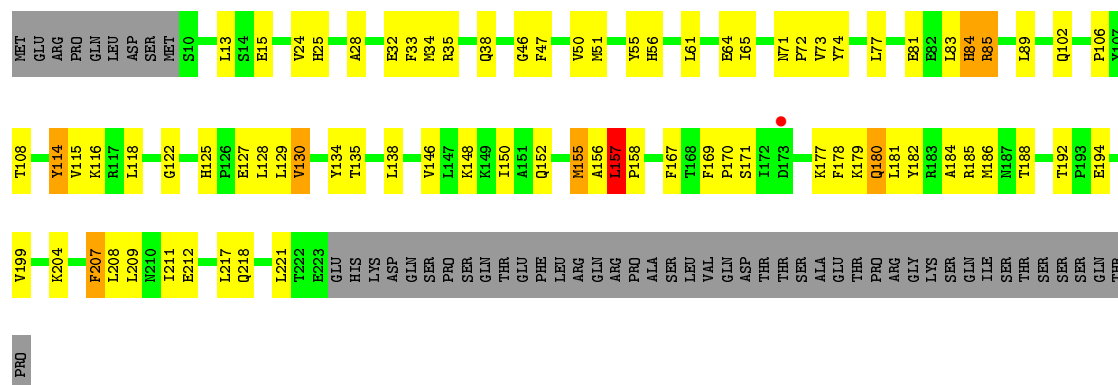
• Molecule 1: NADPH-cytochrome P450 reductase





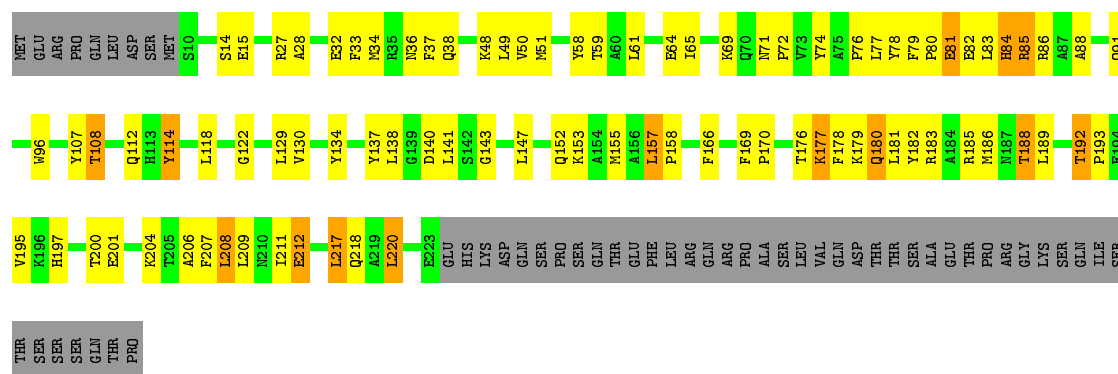
• Molecule 2: Heme oxygenase 1

Chain C: 51% 27% 20%



• Molecule 2: Heme oxygenase 1

Chain D: 47% 28% 5% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	290.34 Å 290.34 Å 83.65 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.34 – 4.30 41.34 – 4.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.34-4.30) 100.0 (41.34-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 4.28 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.222 , 0.256 0.215 , 0.250	Depositor DCC
R_{free} test set	1399 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	165.5	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 168.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.053 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13354	wwPDB-VP
Average B, all atoms (Å ²)	235.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, HEM, NAP, 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	0.56	0/4950	0.83	4/6700 (0.1%)
1	B	0.65	2/4832 (0.0%)	0.87	2/6537 (0.0%)
2	C	0.59	0/1786	0.85	1/2416 (0.0%)
2	D	0.75	0/1786	0.99	2/2416 (0.1%)
All	All	0.63	2/13354 (0.0%)	0.87	9/18069 (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	1
2	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	518	PHE	CG-CD2	6.74	1.48	1.38
1	B	518	PHE	CB-CG	5.93	1.61	1.51

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	648	GLY	N-CA-C	-9.53	89.27	113.10
1	A	648	GLY	N-CA-C	-6.01	98.07	113.10
1	A	662	LEU	CB-CG-CD1	-6.00	100.80	111.00
2	D	181	LEU	CB-CG-CD2	-5.79	101.15	111.00
1	B	326	LEU	CA-CB-CG	5.68	128.37	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	347	LEU	Peptide
2	D	81	GLU	Peptide

5.2 Too-close contacts ⓘ

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	4834	0	4679	177	0
1	B	4720	0	4583	227	0
2	C	1742	0	1712	60	0
2	D	1742	0	1712	83	0
3	A	53	0	31	2	0
3	B	53	0	31	4	0
4	A	31	0	19	4	0
4	B	31	0	19	1	0
5	A	31	0	11	0	0
5	B	31	0	11	4	0
6	C	43	0	30	1	0
6	D	43	0	30	1	0
All	All	13354	0	12868	523	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 20.

The worst 5 of 523 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:CYS:HA	1:B:233:VAL:CG1	1.71	1.20
1:B:201:PHE:CE1	1:B:404:SER:HB2	1.88	1.09
1:B:228:CYS:HA	1:B:233:VAL:HG12	1.33	1.08
1:B:201:PHE:HE1	1:B:404:SER:HB2	0.98	1.05
1:B:398:LEU:HD21	1:B:430:TYR:CD2	1.94	1.02

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	598/618 (97%)	539 (90%)	50 (8%)	9 (2%)	13	58
1	B	582/618 (94%)	509 (88%)	57 (10%)	16 (3%)	6	47
2	C	212/267 (79%)	197 (93%)	13 (6%)	2 (1%)	21	67
2	D	212/267 (79%)	193 (91%)	18 (8%)	1 (0%)	34	77
All	All	1604/1770 (91%)	1438 (90%)	138 (9%)	28 (2%)	11	56

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	VAL
1	A	236	SER
1	A	237	SER
1	A	376	PRO
1	B	230	PHE

5.3.2 Protein sidechains

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	517/528 (98%)	475 (92%)	42 (8%)	15	52
1	B	504/528 (96%)	445 (88%)	59 (12%)	7	35
2	C	183/233 (78%)	164 (90%)	19 (10%)	9	40
2	D	183/233 (78%)	163 (89%)	20 (11%)	8	38
All	All	1387/1522 (91%)	1247 (90%)	140 (10%)	9	41

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	312	SER
1	B	460	VAL
2	D	157	LEU
1	B	318	VAL
1	B	381	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	289	ASN
1	B	380	ASN
2	D	112	GLN
1	B	290	GLN
1	B	298	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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
3	FAD	A	701	-	52,58,58	1.48	8 (15%)	52,89,89	2.71	12 (23%)
4	FMN	A	702	-	32,33,33	1.75	6 (18%)	34,50,50	2.27	7 (20%)
5	NAP	A	703	-	28,33,52	1.19	2 (7%)	35,52,80	2.34	8 (22%)
3	FAD	B	701	-	52,58,58	1.33	5 (9%)	52,89,89	2.85	16 (30%)
4	FMN	B	702	-	32,33,33	1.85	6 (18%)	34,50,50	2.49	8 (23%)
5	NAP	B	703	-	28,33,52	0.97	1 (3%)	35,52,80	3.29	11 (31%)
6	HEM	C	300	-	24,50,50	0.63	0	16,82,82	1.71	4 (25%)
6	HEM	D	300	-	24,50,50	0.80	1 (4%)	16,82,82	2.24	7 (43%)

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
3	FAD	A	701	-	-	0/30/50/50	0/6/6/6
4	FMN	A	702	-	-	0/18/18/18	0/3/3/3
5	NAP	A	703	-	-	0/17/37/67	0/3/3/5
3	FAD	B	701	-	-	0/30/50/50	0/6/6/6
4	FMN	B	702	-	-	0/18/18/18	0/3/3/3
5	NAP	B	703	-	-	0/17/37/67	0/3/3/5
6	HEM	C	300	-	-	0/6/54/54	0/0/8/8
6	HEM	D	300	-	-	0/6/54/54	0/0/8/8

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	300	HEM	C1B-NB	-2.28	1.33	1.36
4	A	702	FMN	C9A-N10	2.07	1.41	1.38
5	B	703	NAP	C5A-C4A	2.12	1.45	1.40
3	A	701	FAD	C4-N3	2.24	1.37	1.33
3	B	701	FAD	C9A-C5X	2.33	1.47	1.42

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	703	NAP	C1B-N9A-C4A	-12.87	112.45	126.81
5	B	703	NAP	N3A-C2A-N1A	-11.20	120.07	128.87
5	A	703	NAP	C1B-N9A-C4A	-9.05	116.71	126.81
3	B	701	FAD	C4-C4X-C10	-7.50	115.14	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	FAD	C4-C4X-C10	-7.09	115.40	119.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	FAD	2	0
4	A	702	FMN	4	0
3	B	701	FAD	4	0
4	B	702	FMN	1	0
5	B	703	NAP	4	0
6	C	300	HEM	1	0
6	D	300	HEM	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	602/618 (97%)	-0.20	4 (0%) 89 84	145, 232, 340, 408	0
1	B	588/618 (95%)	-0.17	14 (2%) 62 52	96, 213, 423, 500	0
2	C	214/267 (80%)	-0.26	1 (0%) 91 88	142, 241, 303, 345	0
2	D	214/267 (80%)	-0.43	0 100 100	114, 180, 251, 294	0
All	All	1618/1770 (91%)	-0.23	19 (1%) 81 73	96, 221, 375, 500	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	152	PHE	5.3
1	B	198	GLN	3.4
1	B	502	ARG	3.2
1	B	206	GLY	3.0
1	A	512	SER	2.9

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, 95th 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(\AA^2)	Q<0.9
6	HEM	D	300	43/43	0.88	0.38	1.57	165,241,289,365	0
6	HEM	C	300	43/43	0.87	0.35	0.30	179,251,316,347	0
5	NAP	B	703	31/48	0.83	0.24	0.21	135,176,209,242	0
3	FAD	B	701	53/53	0.92	0.26	0.07	117,159,213,241	0
5	NAP	A	703	31/48	0.68	0.30	-0.47	154,224,280,288	0
3	FAD	A	701	53/53	0.92	0.24	-0.59	133,190,255,302	0
4	FMN	B	702	31/31	0.94	0.17	-0.86	269,335,425,433	0
4	FMN	A	702	31/31	0.93	0.15	-0.97	245,333,377,395	0

6.5 Other polymers [i](#)

There are no such residues in this entry.