WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 15, 2017 – 01:57 am GMT

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)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

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	Percentile Ranks	Value
Rfree		0.250
Clashscore		20
Ramachandran outliers		1.7%
Sidechain outliers		10.1%
RSRZ outliers		1.2%

Worse   *Better*

▋ Percentile relative to all X-ray structures

❘ Percentile relative to X-ray structures of similar resolution
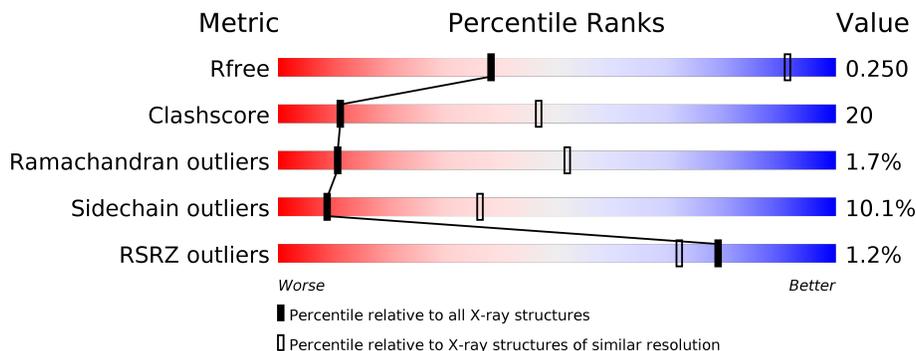
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1002 (4.92-3.62)
Clashscore	112137	1001 (4.92-3.68)
Ramachandran outliers	110173	1012 (4.92-3.64)
Sidechain outliers	110143	1021 (4.92-3.62)
RSRZ outliers	101464	1009 (4.92-3.62)

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	618	% 60% 33% · ·
1	B	618	2% 54% 34% 7% 5%
2	C	267	51% 27% · 20%
2	D	267	47% 28% 5% 20%

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 4834	C 3063	N 830	O 918	S 23	0	0	0
1	B	588	Total 4720	C 2992	N 816	O 889	S 23	0	0	0

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 1742	C 1116	N 298	O 322	S 6	0	0	0
2	D	214	Total 1742	C 1116	N 298	O 322	S 6	0	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).
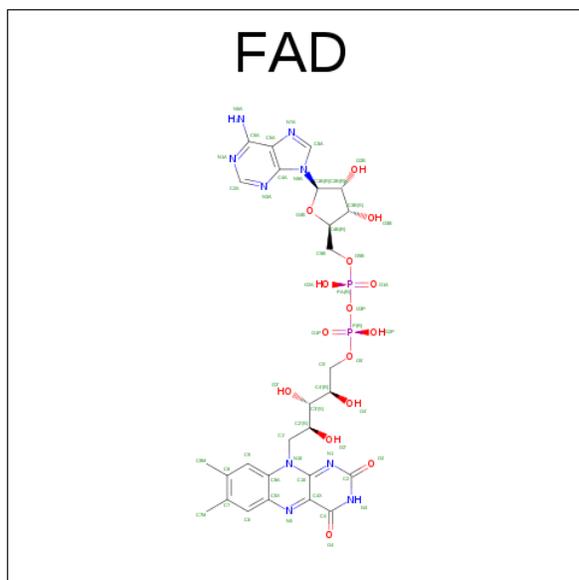
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).
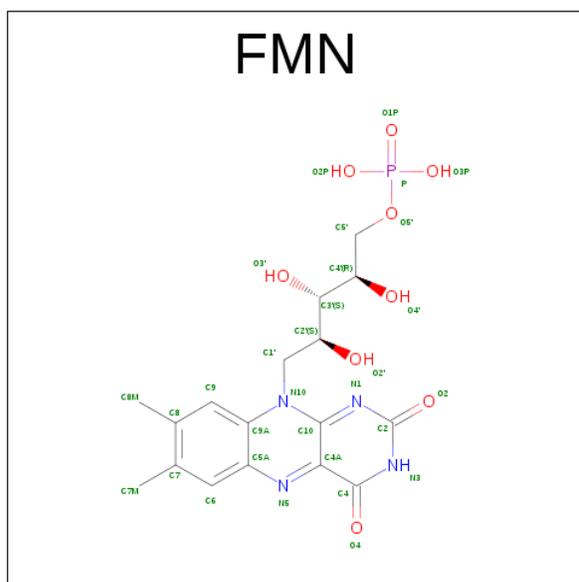
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 5 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).
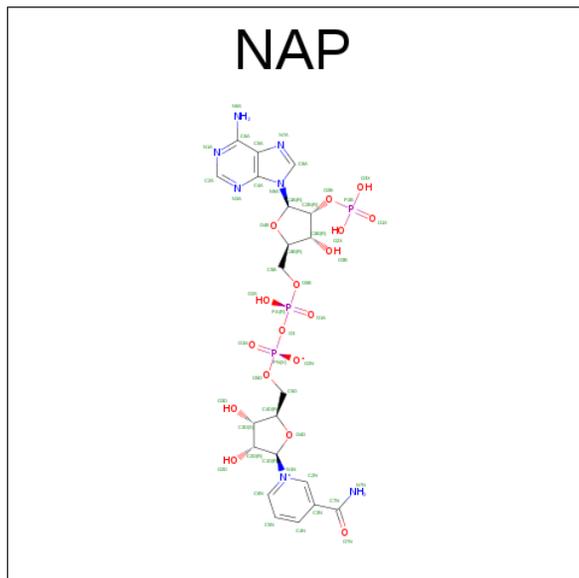
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
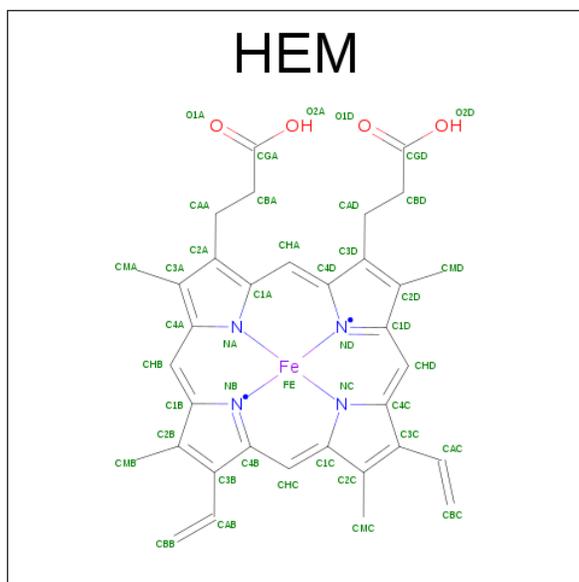
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: NADPH-cytochrome P450 reductase

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P320 A321 N322 L326 V327 I330 D337 L338 D339 V340 I341 M342 S343 L347 D348 E349 E350 K353 P356 F357 P358 C359 P360 T361 R364 L367 I373 T374 N375 P376 P377 R378 T379 N380 V381 E384 Q387 Y388 E391 P392 S393 E394 Q395 E396 H397 L398 A402

S403 S404 E410 L413 E418 A419 R420 R421 H422 A425 D429 Y430 L433 P436 H439 E442 R450 Y451 Y452 S453 I454 V460 I467 V470 A471 V472 E473 Y474 E475 A476 K477 S478 G479 R480 V481 N482 K483 G484 V485 A486 T487 E494 P495 ALA GLY GLU

ASN GLY GLY R502 A503 L504 M507 R510 K511 R515 L516 P517 F518 T521 T522 P523 M526 V527 G528 P529 G530 T531 G532 I533 A534 P535 F536 F539 W545 L546 R547 E648 Q549 G554 E555 T556 Y559 R563 R564 S565 D566 E567 D568 Y569 L570 R577 K580

A583 L584 T585 Q586 L587 N588 F591 S592 R593 E594 Y600 V601 Q602 L605 R609 L612 W613 K614 L615 I616 A621 H622 I623 Y624 G627 D628 A629 M632 D635 V636 Q637 N638 T639 F640 Y641 V644 F647 G648 P649 A655 V656 D657 Y658 V659 K660 K661 L662 M663

T664 K665 G666 R667 Y668 S669 L670 D671 V672 W673 S674

• Molecule 2: Heme oxygenase 1

Chain C:

51%   27%   •   20%

MET GLU ARG PRO GLN LEU ASP SER MET S10 L13 S14 E15 V24 H25 A28 E32 F33 M34 R35 Q38 G46 F47 V50 M51 Y55 H56 L61 E64 I65 N71 P72 V73 Y74 L77 E81 E82 L83 H84 R85 L89 Q102 P106 Y107

T108 Y114 V115 K116 R117 L118 G122 H125 P126 E127 L128 L129 V130 Y134 T135 L138 V146 L147 K148 K149 I150 A151 Q152 M155 A156 L157 P158 F167 T168 F169 P170 S171 I172 D173 K177 F178 K179 Q180 L181 Y182 R183 A184 R185 M186 N187 T188 T192 P193 E194

V199 K204 F207 L208 L209 N210 I211 E212 L217 Q218 L221 T222 E223 GLU HIS LYS ASP SER PRO SER GLN THR GLU PHE LEU ARG GLN ARG PRO ALA SER LEU VAL GLN ASP THR THR SER ALA GLU THR PRO ARG GLY LYS SER GLN ILE SER SER SER GLN THR

PRO

• Molecule 2: Heme oxygenase 1

Chain D:

47%   28%   5%   20%

MET GLU ARG PRO GLN LEU ASP SER MET S10 S14 E15 R27 A28 E32 F33 M34 R35 N36 F37 Q38 K48 L49 V50 M51 Y58 T59 A60 L61 E64 I65 K69 Q70 N71 P72 V73 Y74 A75 P76 L77 Y78 F79 P80 E81 E82 L83 H84 R85 R86 A87 A88 Q91

W96 Y107 T108 Q112 H113 Y114 L118 G122 L129 V130 Y134 Y137 L138 G139 D140 L141 S142 G143 L147 Q152 K153 A154 M155 A156 L157 P158 F166 F169 P170 T176 K177 F178 K179 Q180 L181 Y182 R183 A184 R185 M186 N187 T188 L189 T192 P193 E194

V195 K196 H197 T200 E201 K204 T205 A206 F207 L208 L209 N210 I211 E212 L217 Q218 A219 L220 E223 GLU HIS LYS ASP SER PRO SER GLN THR GLU PHE LEU ARG GLN ARG PRO ALA SER LEU VAL GLN ASP THR THR SER ALA GLU THR PRO ARG GLY LYS SER GLN ILE SER

THR SER SER SER GLN THR PRO

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	290.34Å 290.34Å 83.65Å 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
$<I/\sigma(I)>$ [1]	3.24 (at 4.28Å)	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 (Å²)	165.5	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.25 , 168.4	EDS
L-test for twinning[2]	$<|L|> = 0.45, <L^2> = 0.28$	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 (Å²)	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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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%)	12	54
1	B	582/618 (94%)	509 (88%)	57 (10%)	16 (3%)	6	42
2	C	212/267 (79%)	197 (93%)	13 (6%)	2 (1%)	20	63
2	D	212/267 (79%)	193 (91%)	18 (8%)	1 (0%)	32	74
All	All	1604/1770 (91%)	1438 (90%)	138 (9%)	28 (2%)	11	52

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%)	14	47
1	B	504/528 (96%)	445 (88%)	59 (12%)	6	31
2	C	183/233 (78%)	164 (90%)	19 (10%)	8	35
2	D	183/233 (78%)	163 (89%)	20 (11%)	7	33
All	All	1387/1522 (91%)	1247 (90%)	140 (10%)	9	36

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   ⓘ

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   ⓘ

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	-	51,58,58	1.55	8 (15%)	54,89,89	2.45	12 (22%)
4	FMN	A	702	-	31,33,33	1.80	6 (19%)	38,50,50	2.12	6 (15%)
5	NAP	A	703	-	28,33,52	1.23	3 (10%)	32,52,80	2.14	8 (25%)
3	FAD	B	701	-	51,58,58	1.40	7 (13%)	54,89,89	2.67	16 (29%)
4	FMN	B	702	-	31,33,33	1.93	5 (16%)	38,50,50	2.39	7 (18%)
5	NAP	B	703	-	28,33,52	0.99	1 (3%)	32,52,80	2.78	10 (31%)
6	HEM	C	300	-	28,50,50	0.68	0	17,82,82	1.35	2 (11%)
6	HEM	D	300	-	28,50,50	0.83	1 (3%)	17,82,82	1.94	5 (29%)

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	-	-	0/28/50/50	0/6/6/6
4	FMN	A	702	-	-	0/16/18/18	0/3/3/3
5	NAP	A	703	-	-	0/17/37/67	0/3/3/5
3	FAD	B	701	-	-	0/28/50/50	0/6/6/6
4	FMN	B	702	-	-	0/16/18/18	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 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	300	HEM	C1B-NB	-2.60	1.33	1.36
5	A	703	NAP	O4B-C1B	2.01	1.44	1.41
3	B	701	FAD	C10-N1	2.07	1.36	1.33
3	B	701	FAD	C2A-N3A	2.08	1.35	1.32
4	A	702	FMN	C4A-N5	2.12	1.36	1.33

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	703	NAP	N3A-C2A-N1A	-10.09	120.07	128.86
5	B	703	NAP	C1B-N9A-C4A	-8.21	112.45	126.64
3	A	701	FAD	N3A-C2A-N1A	-6.20	123.46	128.86
3	B	701	FAD	C4-C4X-C10	-5.96	115.14	119.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	703	NAP	C1B-N9A-C4A	-5.75	116.71	126.64

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 ⓘ

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, 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%)	87	82	145, 232, 340, 408	0
1	B	588/618 (95%)	-0.17	14 (2%)	59	51	96, 213, 423, 500	0
2	C	214/267 (80%)	-0.26	1 (0%)	90	86	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%)	79	72	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 ⓘ

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

6.3 Carbohydrates ⓘ

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, 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($Å^2$)	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	0.06	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	-0.87	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 ⓘ

There are no such residues in this entry.