



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:28 PM UTC

PDB ID : 6MCW / pdb_00006mcw
Title : Crystal structure of the P450 domain of the CYP51-ferredoxin fusion protein from *Methylococcus capsulatus*, complex with the detergent Anapoe-X-114
Authors : Hargrove, T.; Wawrzak, Z.; Lamb, D.C.; Lepesheva, G.I.
Deposited on : 2018-09-02
Resolution : 2.40 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

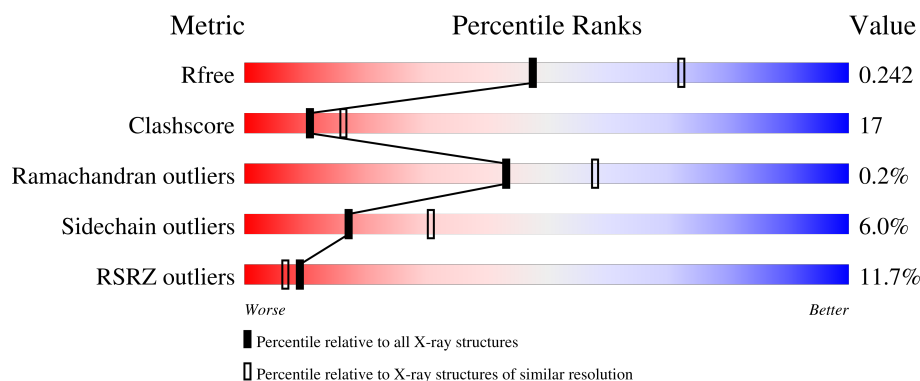
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	551	9% 60% 18% • 19%

2 Entry composition [i](#)

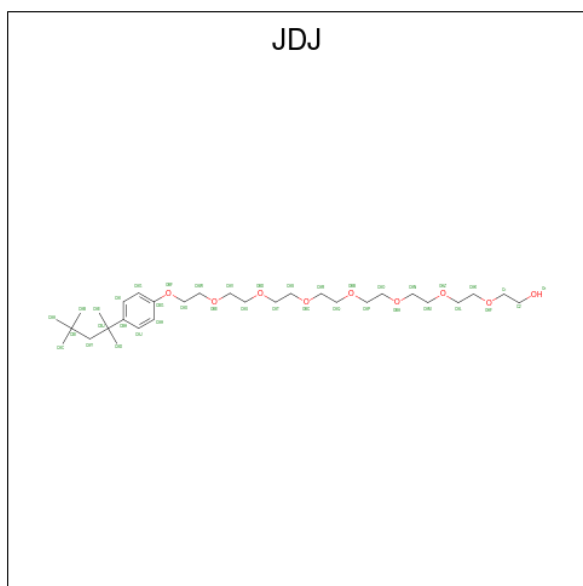
There are 4 unique types of molecules in this entry. The entry contains 3724 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cytochrome P450 51.

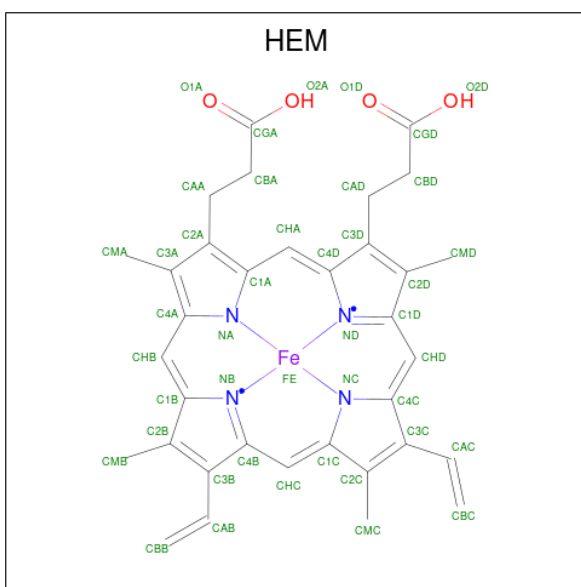
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	446	3609	2301	644	641	23	0	0	0

- Molecule 2 is 23-[4-(2,4,4-trimethylpentan-2-yl)phenoxy]-3,6,9,12,15,18,21-heptaooxatricosan-1-ol (CCD ID: JDJ) (formula: C₃₀H₅₄O₉).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	36	28	8	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	36	Total O 36 36	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.69Å 150.69Å 66.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.96 – 2.40 29.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.96-2.40) 99.2 (29.96-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.216 , 0.237 0.227 , 0.242	Depositor DCC
R_{free} test set	1673 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3724	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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, 0.333 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: JDJ, HEM

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	0.54	2/3695 (0.1%)	0.99	7/4996 (0.1%)

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	440	PRO	C-O	-6.11	1.19	1.24
1	A	277	PRO	C-O	-5.32	1.17	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	PRO	N-CA-C	-10.39	101.73	114.20
1	A	13	PRO	CA-C-N	7.70	129.76	120.14
1	A	13	PRO	C-N-CA	7.70	129.76	120.14
1	A	14	GLY	N-CA-C	6.93	122.31	113.24
1	A	91	VAL	CA-C-N	5.26	134.19	124.82
1	A	91	VAL	C-N-CA	5.26	134.19	124.82
1	A	440	PRO	N-CA-C	-5.13	102.23	110.74

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	ARG	Sidechain

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	3609	0	3621	117	0
2	A	36	0	0	7	0
3	A	43	0	30	6	0
4	A	36	0	0	2	0
All	All	3724	0	3651	122	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 17.

All (122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LEU:HG	1:A:194:PRO:HD2	1.30	1.12
1:A:193:LEU:CG	1:A:194:PRO:HD2	1.92	0.98
1:A:184:ILE:O	1:A:188:PHE:HD2	1.54	0.90
2:A:601:JDJ:CAD	4:A:701:HOH:O	2.21	0.88
1:A:92:PHE:HE2	2:A:601:JDJ:CAB	1.87	0.86
1:A:191:LEU:H	1:A:192:PRO:CD	1.89	0.84
1:A:193:LEU:HG	1:A:194:PRO:CD	2.07	0.84
2:A:601:JDJ:CAE	2:A:601:JDJ:CAC	2.54	0.84
1:A:92:PHE:CE2	2:A:601:JDJ:CAB	2.61	0.84
1:A:184:ILE:HB	1:A:188:PHE:CE2	2.13	0.83
1:A:188:PHE:HB3	1:A:190:ASN:HB2	1.62	0.82
1:A:191:LEU:H	1:A:192:PRO:HD3	1.44	0.82
3:A:602:HEM:HMC2	3:A:602:HEM:HBC2	1.62	0.81
1:A:88:ARG:HA	1:A:93:ASP:OD2	1.80	0.81
1:A:371:TYR:CD1	1:A:377:GLU:HG2	2.21	0.76
1:A:290:LEU:HD13	1:A:301:SER:HB2	1.67	0.75
1:A:371:TYR:HD1	1:A:377:GLU:HG2	1.51	0.75
1:A:242:LEU:HD13	1:A:250:MET:HE1	1.70	0.74
1:A:184:ILE:O	1:A:188:PHE:CD2	2.40	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ALA:HB2	2:A:601:JDJ:CAA	2.19	0.72
1:A:381:LEU:O	1:A:381:LEU:HD23	1.88	0.72
1:A:184:ILE:HB	1:A:188:PHE:HE2	1.54	0.71
1:A:299:PHE:CE2	1:A:303:ARG:HD2	2.25	0.70
1:A:128:ALA:HA	1:A:131:ARG:HH11	1.57	0.70
1:A:419:LEU:HD23	1:A:443:ILE:HD11	1.77	0.67
1:A:90:VAL:HG12	1:A:91:VAL:H	1.60	0.66
1:A:203:ARG:HG3	1:A:203:ARG:HH11	1.61	0.66
1:A:188:PHE:C	1:A:190:ASN:H	2.03	0.66
1:A:242:LEU:HD22	1:A:250:MET:HE1	1.77	0.66
1:A:157:LEU:HD13	1:A:254:THR:HG22	1.77	0.65
1:A:188:PHE:HB3	1:A:190:ASN:CB	2.28	0.64
1:A:16:LEU:HD23	1:A:19:LEU:HD12	1.79	0.63
1:A:90:VAL:HG12	1:A:91:VAL:N	2.13	0.63
1:A:188:PHE:CB	1:A:190:ASN:HB2	2.29	0.62
1:A:298:THR:HG22	1:A:301:SER:H	1.64	0.62
1:A:429:ASP:OD2	1:A:432:LYS:HE3	2.00	0.62
1:A:9:PRO:HB3	1:A:43:VAL:HG12	1.82	0.62
1:A:189:PRO:CD	1:A:190:ASN:N	2.61	0.61
1:A:418:GLU:OE2	1:A:444:ARG:NH1	2.33	0.61
1:A:193:LEU:CD2	1:A:194:PRO:HD2	2.31	0.61
1:A:272:GLU:OE2	1:A:276:ARG:NH1	2.32	0.61
1:A:85:ILE:O	1:A:203:ARG:HD3	2.00	0.60
1:A:153:SER:O	1:A:157:LEU:HG	2.01	0.59
1:A:290:LEU:CD1	1:A:301:SER:HB2	2.31	0.59
1:A:191:LEU:N	1:A:192:PRO:CD	2.58	0.59
1:A:419:LEU:HD23	1:A:443:ILE:CD1	2.32	0.59
1:A:22:ILE:HD13	1:A:49:PHE:CZ	2.37	0.59
1:A:376:ALA:HB1	1:A:379:LYS:HG2	1.83	0.59
1:A:298:THR:HG23	1:A:300:GLU:H	1.66	0.58
1:A:199:ARG:HD2	1:A:200:ASP:OD1	2.03	0.58
1:A:206:LEU:CD2	1:A:252:ILE:HD11	2.34	0.58
1:A:128:ALA:HA	1:A:131:ARG:NH1	2.19	0.57
1:A:189:PRO:HD2	1:A:190:ASN:N	2.20	0.56
1:A:193:LEU:HB2	1:A:196:PHE:CD2	2.40	0.56
1:A:90:VAL:CG1	1:A:91:VAL:H	2.18	0.56
1:A:139:ILE:HG12	1:A:443:ILE:HG22	1.88	0.55
3:A:602:HEM:HBC2	3:A:602:HEM:CMC	2.36	0.54
1:A:90:VAL:O	1:A:91:VAL:C	2.51	0.54
1:A:242:LEU:CD1	1:A:250:MET:HE1	2.38	0.54
1:A:400:ALA:HB1	3:A:602:HEM:HBB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ARG:NH1	1:A:300:GLU:OE2	2.42	0.52
1:A:16:LEU:N	1:A:16:LEU:CD1	2.72	0.52
1:A:188:PHE:C	1:A:190:ASN:N	2.67	0.52
1:A:184:ILE:HB	1:A:188:PHE:CD2	2.46	0.51
1:A:90:VAL:CG1	1:A:91:VAL:N	2.74	0.51
1:A:191:LEU:O	1:A:196:PHE:CD2	2.64	0.51
1:A:257:ALA:CB	2:A:601:JDJ:CAA	2.88	0.50
1:A:416:GLU:HG3	1:A:446:ARG:HH21	1.77	0.50
1:A:282:ARG:NH2	1:A:369:ASP:OD1	2.43	0.50
1:A:184:ILE:C	1:A:188:PHE:HD2	2.16	0.49
1:A:206:LEU:HD22	1:A:252:ILE:HD11	1.93	0.49
3:A:602:HEM:HBB2	3:A:602:HEM:HHC	1.94	0.49
1:A:20:GLY:HA3	1:A:47:ARG:O	2.12	0.49
1:A:332:ASP:OD2	1:A:339:ARG:NH1	2.45	0.49
1:A:16:LEU:N	1:A:16:LEU:HD12	2.27	0.48
1:A:299:PHE:O	1:A:303:ARG:HG3	2.13	0.48
1:A:419:LEU:HD22	1:A:426:TYR:CZ	2.48	0.48
1:A:272:GLU:OE2	1:A:272:GLU:HA	2.14	0.48
1:A:189:PRO:HD2	1:A:190:ASN:CG	2.38	0.48
1:A:188:PHE:HB3	1:A:190:ASN:H	1.78	0.48
1:A:189:PRO:CD	1:A:190:ASN:H	2.27	0.47
1:A:95:ARG:O	1:A:96:ILE:C	2.57	0.47
1:A:89:GLY:H	1:A:93:ASP:CG	2.23	0.47
1:A:324:LEU:HD11	1:A:347:CYS:SG	2.55	0.47
1:A:158:LEU:HD21	1:A:255:ILE:HD11	1.96	0.47
1:A:242:LEU:CD2	1:A:250:MET:HE1	2.42	0.47
1:A:114:PRO:HB3	1:A:230:MET:HE1	1.96	0.47
1:A:257:ALA:HA	2:A:601:JDJ:CAD	2.46	0.46
1:A:8:THR:HB	1:A:9:PRO:HD2	1.96	0.46
1:A:330:MET:HE2	1:A:330:MET:HA	1.97	0.46
1:A:417:PHE:HA	1:A:444:ARG:O	2.17	0.45
1:A:111:ARG:O	1:A:114:PRO:HD2	2.16	0.45
1:A:288:ASP:O	1:A:292:GLU:HG2	2.17	0.44
1:A:193:LEU:HB2	1:A:196:PHE:HD2	1.79	0.44
1:A:53:MET:HE2	1:A:347:CYS:SG	2.58	0.44
1:A:81:ILE:HB	1:A:186:TYR:HB2	2.00	0.44
1:A:193:LEU:CB	1:A:196:PHE:CD2	3.01	0.43
1:A:53:MET:HE1	1:A:347:CYS:HB3	1.99	0.43
1:A:188:PHE:CD1	1:A:190:ASN:ND2	2.86	0.43
1:A:147:GLU:O	1:A:150:ILE:HG22	2.18	0.43
1:A:284:ARG:NH2	1:A:415:TYR:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:THR:N	1:A:84:PRO:CD	2.82	0.43
1:A:325:LEU:O	1:A:347:CYS:HA	2.18	0.43
1:A:292:GLU:HG2	1:A:292:GLU:H	1.72	0.43
1:A:188:PHE:CB	1:A:190:ASN:H	2.32	0.43
1:A:223:ARG:O	1:A:223:ARG:HG3	2.18	0.43
1:A:107:MET:N	1:A:108:PRO:HD2	2.34	0.43
1:A:396:GLY:HA3	3:A:602:HEM:C3C	2.54	0.43
1:A:80:ARG:HD3	1:A:80:ARG:HA	1.80	0.42
1:A:166:LEU:CD1	1:A:213:ILE:HD11	2.50	0.41
1:A:188:PHE:HD1	1:A:190:ASN:ND2	2.18	0.41
1:A:193:LEU:CB	1:A:194:PRO:HD2	2.50	0.41
1:A:242:LEU:HD22	1:A:250:MET:CE	2.49	0.41
1:A:277:PRO:O	1:A:281:ARG:HG3	2.20	0.41
1:A:191:LEU:O	1:A:196:PHE:CG	2.74	0.41
1:A:400:ALA:HB1	3:A:602:HEM:CBB	2.51	0.41
1:A:419:LEU:HD22	1:A:426:TYR:CE1	2.56	0.41
1:A:23:LEU:HB2	4:A:712:HOH:O	2.21	0.41
1:A:191:LEU:N	1:A:192:PRO:HD3	2.14	0.41
1:A:157:LEU:HD13	1:A:254:THR:CG2	2.46	0.41
1:A:268:TRP:CE2	1:A:437:PRO:HG3	2.56	0.41
1:A:314:GLU:OE1	1:A:314:GLU:HA	2.21	0.41

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	444/551 (81%)	424 (96%)	19 (4%)	1 (0%)	43 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	LEU

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	386/466 (83%)	363 (94%)	23 (6%)	17	31

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	MET
1	A	85	ILE
1	A	97	GLU
1	A	148	LEU
1	A	165	GLU
1	A	187	VAL
1	A	189	PRO
1	A	193	LEU
1	A	235	SER
1	A	284	ARG
1	A	290	LEU
1	A	292	GLU
1	A	298	THR
1	A	304	GLN
1	A	309	GLU
1	A	330	MET
1	A	335	VAL
1	A	346	VAL
1	A	377	GLU
1	A	379	LYS
1	A	412	LEU
1	A	439	SER
1	A	443	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	102	GLN
1	A	201	GLN
1	A	212	GLN
1	A	260	HIS
1	A	294	HIS
1	A	304	GLN
1	A	385	GLN
1	A	414	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	JDJ	A	601	-	36,36,39	1.59	1 (2%)	44,44,47	1.00	2 (4%)
3	HEM	A	602	1,4	50,50,50	1.59	10 (20%)	67,82,82	1.75	16 (23%)

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	JDJ	A	601	-	-	17/34/34/37	0/1/1/1
3	HEM	A	602	1,4	-	2/14/54/54	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	JDJ	CBJ-CBH	-9.08	1.39	1.53
3	A	602	HEM	FE-NB	5.06	2.10	1.94
3	A	602	HEM	FE-NC	4.25	2.09	1.95
3	A	602	HEM	C1B-NB	-3.52	1.34	1.40
3	A	602	HEM	C4D-ND	-3.43	1.34	1.40
3	A	602	HEM	FE-ND	-2.87	1.86	1.94
3	A	602	HEM	C1D-ND	-2.33	1.34	1.38
3	A	602	HEM	C3B-C4B	2.19	1.49	1.44
3	A	602	HEM	C4B-NB	-2.15	1.34	1.38
3	A	602	HEM	C1C-C2C	-2.10	1.41	1.45
3	A	602	HEM	C3C-C4C	-2.10	1.42	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	HEM	CHB-C1B-NB	4.92	130.46	124.37
3	A	602	HEM	CHA-C4D-ND	4.22	129.59	124.37
3	A	602	HEM	CHD-C1D-ND	4.13	128.86	124.42
2	A	601	JDJ	CAY-CBJ-CBH	-4.08	102.45	112.00
3	A	602	HEM	CHC-C4B-NB	3.76	128.47	124.42
3	A	602	HEM	CHA-C4D-C3D	-3.50	118.77	125.23
3	A	602	HEM	CHD-C1D-C2D	-3.24	119.91	125.03
3	A	602	HEM	C1B-NB-C4B	3.15	108.93	105.21
2	A	601	JDJ	CAI-CBH-CBJ	-3.02	116.06	121.52
3	A	602	HEM	CHD-C4C-NC	2.87	127.58	124.45
3	A	602	HEM	CHB-C1B-C2B	-2.78	119.05	126.95
3	A	602	HEM	CAB-C3B-C2B	-2.48	120.36	128.43
3	A	602	HEM	C1A-CHA-C4D	-2.37	120.68	126.25
3	A	602	HEM	C3B-C4B-NB	-2.36	107.78	109.47
3	A	602	HEM	O2D-CGD-CBD	2.18	120.89	114.00
3	A	602	HEM	C4C-CHD-C1D	-2.15	121.45	126.02
3	A	602	HEM	CAB-C3B-C4B	2.15	133.87	124.39
3	A	602	HEM	CMD-C2D-C1D	2.04	128.22	125.03

There are no chirality outliers.

All (19) torsion outliers are listed below:

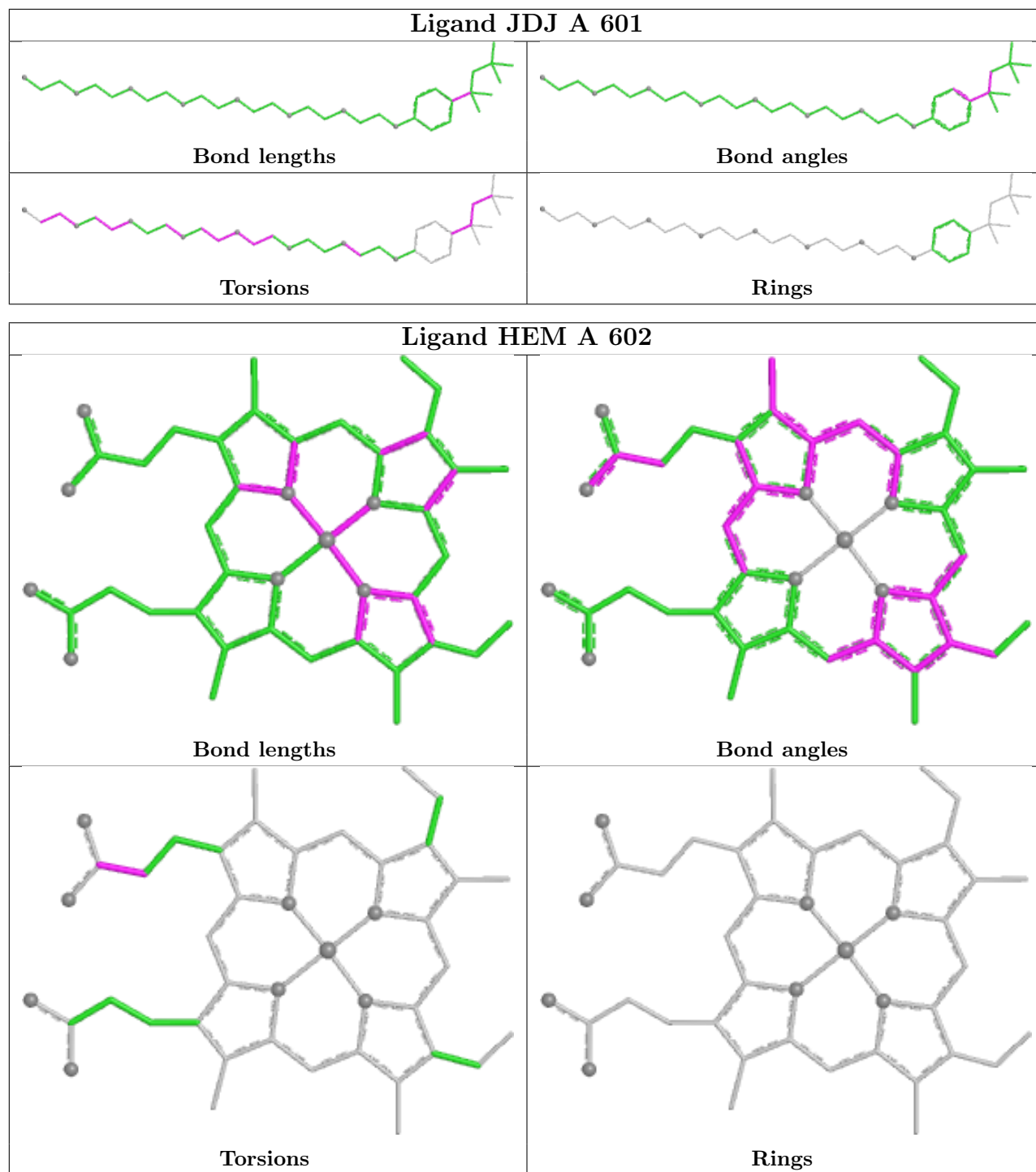
Mol	Chain	Res	Type	Atoms
2	A	601	JDJ	CBJ-CAY-CBI-CAC
2	A	601	JDJ	CAM-CAN-OBA-CAO
2	A	601	JDJ	CBJ-CAY-CBI-CAB
2	A	601	JDJ	CBJ-CAY-CBI-CAA
2	A	601	JDJ	OAF-CAK-CAL-OAZ
2	A	601	JDJ	CAX-CAW-OBE-CAV
2	A	601	JDJ	CAK-CAL-OAZ-CAM
2	A	601	JDJ	CAI-CBH-CBJ-CAY
2	A	601	JDJ	CAO-CAP-OBB-CAQ
2	A	601	JDJ	OBC-CAS-CAT-OBD
2	A	601	JDJ	CAT-CAS-OBC-CAR
2	A	601	JDJ	CAI-CBH-CBJ-CAE
3	A	602	HEM	CAD-CBD-CGD-O1D
3	A	602	HEM	CAD-CBD-CGD-O2D
2	A	601	JDJ	OBB-CAQ-CAR-OBC
2	A	601	JDJ	CBI-CAY-CBJ-CBH
2	A	601	JDJ	CAQ-CAR-OBC-CAS
2	A	601	JDJ	CAI-CBH-CBJ-CAD
2	A	601	JDJ	OAZ-CAM-CAN-OBA

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	JDJ	7	0
3	A	602	HEM	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	446/551 (80%)	0.48	52 (11%) 9 7	33, 53, 101, 185	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	187	VAL	11.4
1	A	191	LEU	8.6
1	A	4	PRO	7.9
1	A	186	TYR	7.4
1	A	379	LYS	6.8
1	A	18	LEU	6.3
1	A	17	PRO	5.3
1	A	192	PRO	5.2
1	A	376	ALA	5.2
1	A	439	SER	5.2
1	A	189	PRO	5.2
1	A	188	PHE	5.2
1	A	47	ARG	4.8
1	A	378	ASP	4.8
1	A	190	ASN	4.6
1	A	184	ILE	4.4
1	A	91	VAL	4.3
1	A	193	LEU	4.1
1	A	5	PRO	4.0
1	A	219	ARG	4.0
1	A	185	ALA	3.9
1	A	79	TYR	3.8
1	A	169	GLU	3.8
1	A	381	LEU	3.7
1	A	290	LEU	3.5
1	A	296	ARG	3.4
1	A	380	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	377	GLU	3.2
1	A	80	ARG	3.1
1	A	131	ARG	3.1
1	A	194	PRO	3.1
1	A	92	PHE	3.1
1	A	14	GLY	3.0
1	A	440	PRO	2.9
1	A	449	ASP	2.8
1	A	221	GLN	2.8
1	A	196	PHE	2.7
1	A	15	GLY	2.7
1	A	183	PRO	2.7
1	A	50	HIS	2.6
1	A	220	SER	2.5
1	A	113	LYS	2.4
1	A	6	SER	2.4
1	A	93	ASP	2.3
1	A	197	LYS	2.2
1	A	303	ARG	2.2
1	A	135	ASP	2.2
1	A	281	ARG	2.1
1	A	446	ARG	2.1
1	A	95	ARG	2.1
1	A	222	GLU	2.1
1	A	292	GLU	2.0

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

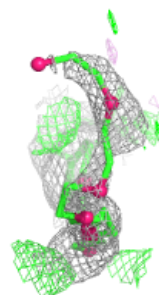
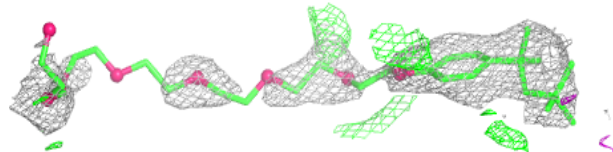
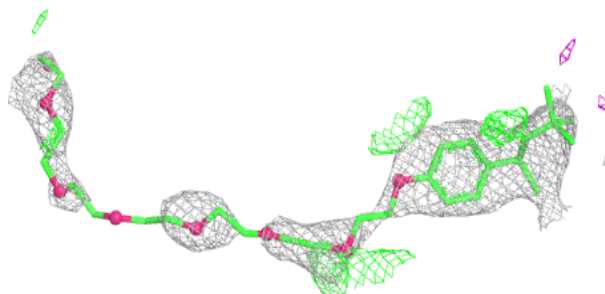
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

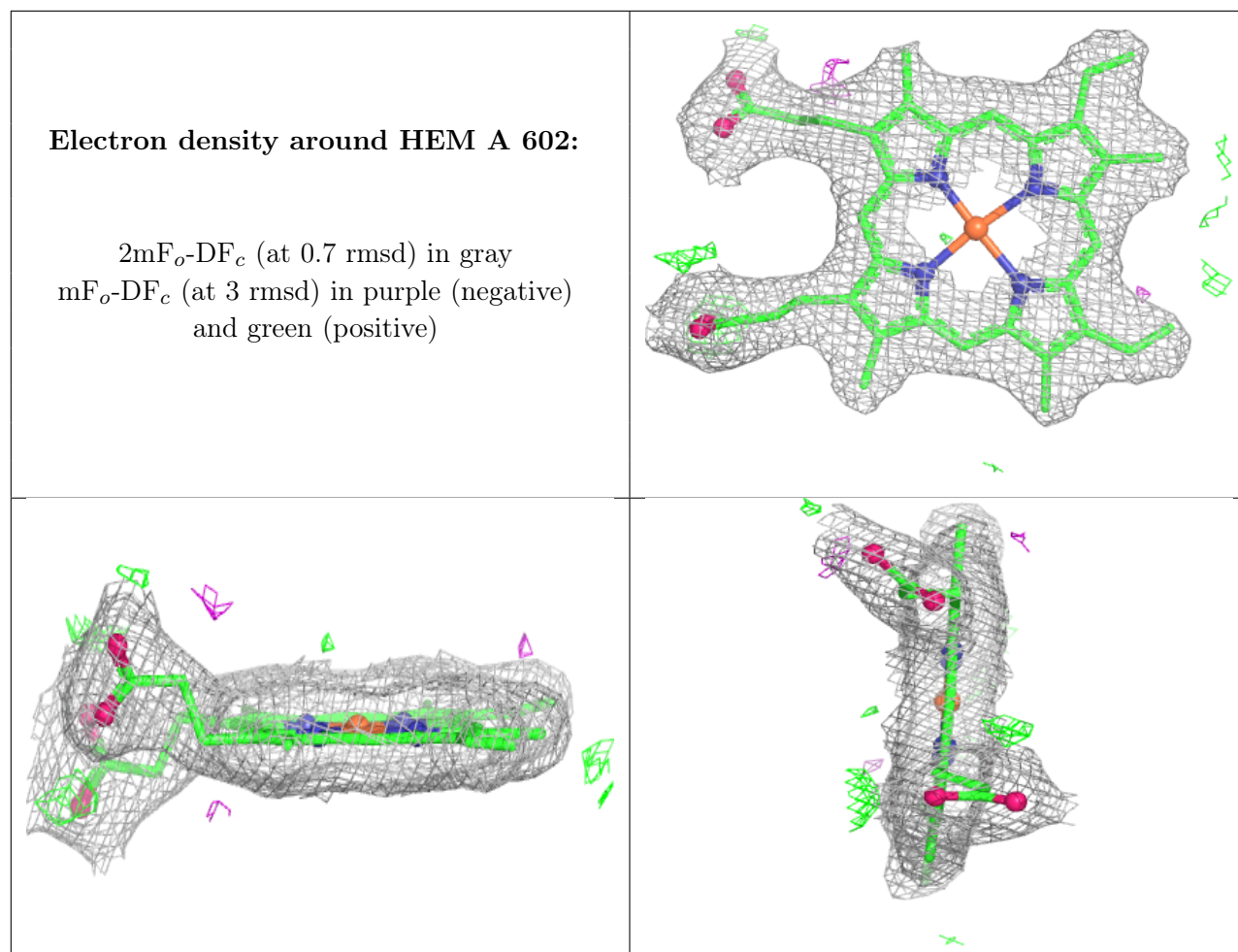
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	JDJ	A	601	36/39	0.81	0.25	81,112,128,130	0
3	HEM	A	602	43/43	0.99	0.06	37,41,48,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around JDJ A 601:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.