



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 16, 2016 – 12:04 AM EDT

PDB ID : 5E58
Title : Crystal Structure Of Cytochrome P450 2B35 from Desert Woodrat Neotoma
Lepida in complex with 4-(4-chlorophenyl)imidazole
Authors : Shah, M.B.; Stout, C.D.; Halpert, J.R.
Deposited on : 2015-10-08
Resolution : 2.40 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-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

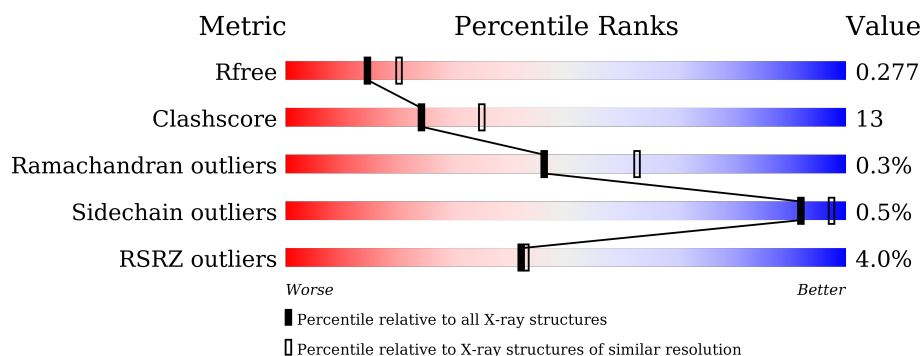
1 Overall quality at a glance ⓘ

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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 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	493	<div> <div>2%</div> <div>83% 11% 6%</div> </div>
1	B	493	<div> <div>5%</div> <div>71% 22% 7%</div> </div>
1	C	493	<div> <div>%</div> <div>75% 19% 6%</div> </div>
1	D	493	<div> <div>3%</div> <div>79% 15% 6%</div> </div>
1	E	493	<div> <div>3%</div> <div>74% 19% 6%</div> </div>
1	F	493	<div> <div>8%</div> <div>67% 24% 7%</div> </div>

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
3	CPZ	A	502	-	-	X	-
3	CPZ	B	502	-	-	X	-
3	CPZ	B	503	-	-	X	-
3	CPZ	C	502	-	-	X	-
3	CPZ	D	502	-	-	X	-
3	CPZ	E	502	-	-	X	-
3	CPZ	F	502	-	-	X	-
3	CPZ	F	503	-	-	X	-
4	SUC	A	504	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23024 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.

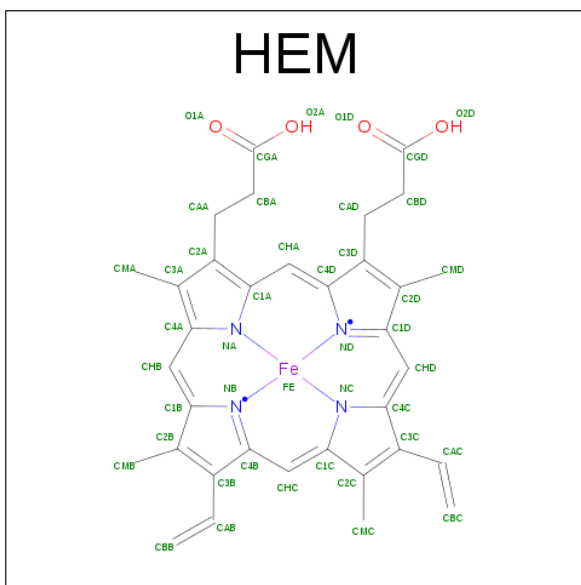
- Molecule 1 is a protein called Cytochrome P450 family 2 subfamily B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3727	2396	638	677	16			
1	B	458	Total	C	N	O	S	0	0	0
			3602	2321	607	659	15			
1	C	465	Total	C	N	O	S	0	0	0
			3685	2371	631	667	16			
1	D	463	Total	C	N	O	S	0	0	0
			3665	2360	623	666	16			
1	E	462	Total	C	N	O	S	0	0	0
			3661	2352	626	667	16			
1	F	458	Total	C	N	O	S	0	1	0
			3558	2284	608	651	15			

There are 12 discrepancies between the modelled and reference sequences:

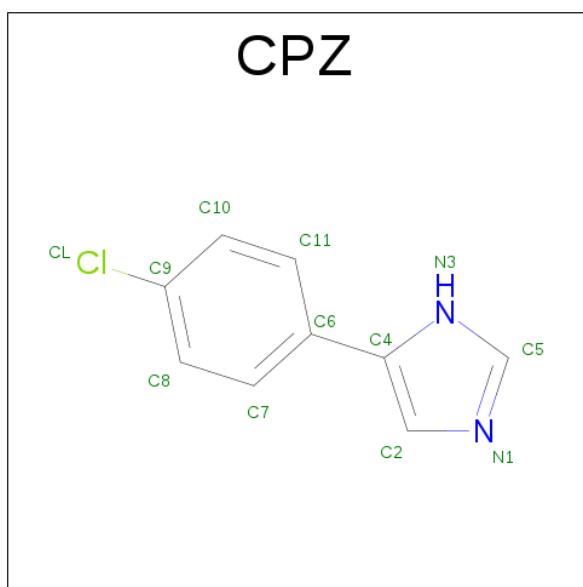
Chain	Residue	Modelled	Actual	Comment	Reference
A	492	HIS	-	expression tag	UNP J9JD66
A	493	HIS	-	expression tag	UNP J9JD66
B	492	HIS	-	expression tag	UNP J9JD66
B	493	HIS	-	expression tag	UNP J9JD66
C	492	HIS	-	expression tag	UNP J9JD66
C	493	HIS	-	expression tag	UNP J9JD66
D	492	HIS	-	expression tag	UNP J9JD66
D	493	HIS	-	expression tag	UNP J9JD66
E	492	HIS	-	expression tag	UNP J9JD66
E	493	HIS	-	expression tag	UNP J9JD66
F	492	HIS	-	expression tag	UNP J9JD66
F	493	HIS	-	expression tag	UNP J9JD66

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



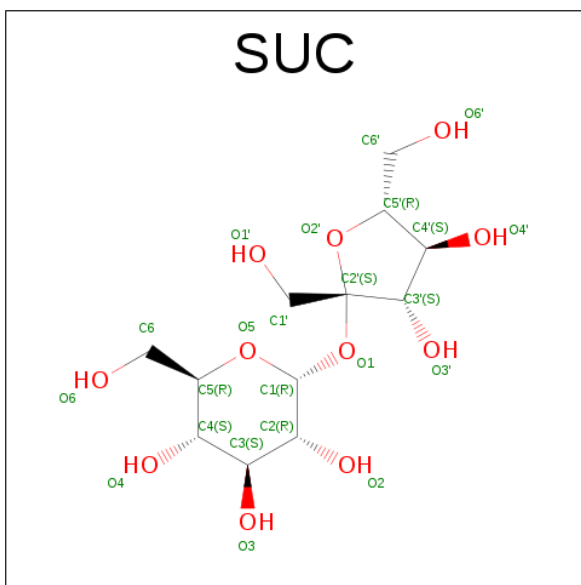
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 4-(4-CHLOROPHENYL)IMIDAZOLE (three-letter code: CPZ) (formula: $C_9H_7ClN_2$).



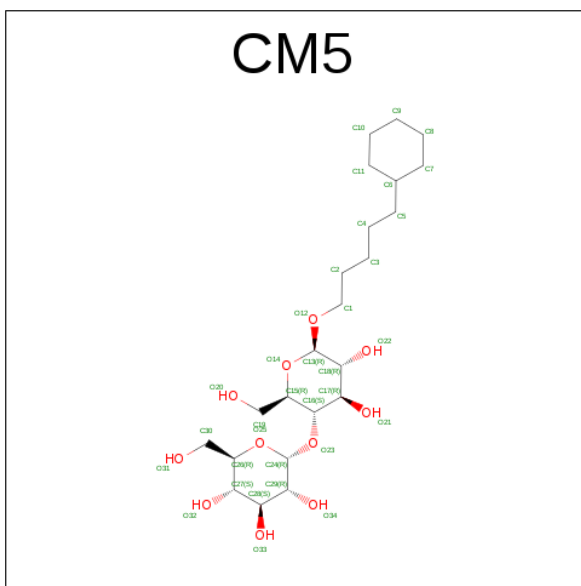
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			12	9	1	2		
3	A	1	Total	C	Cl	N	0	0
			12	9	1	2		
3	B	1	Total	C	Cl	N	0	0
			12	9	1	2		
3	B	1	Total	C	Cl	N	0	0
			12	9	1	2		
3	C	1	Total	C	Cl	N	0	0
			12	9	1	2		
3	C	1	Total	C	Cl	N	0	0
			12	9	1	2		
3	D	1	Total	C	Cl	N	0	0
			12	9	1	2		
3	D	1	Total	C	Cl	N	0	0
			12	9	1	2		
3	E	1	Total	C	Cl	N	0	0
			12	9	1	2		
3	E	1	Total	C	Cl	N	0	0
			12	9	1	2		
3	F	1	Total	C	Cl	N	0	0
			12	9	1	2		
3	F	1	Total	C	Cl	N	0	0
			12	9	1	2		

- Molecule 4 is SUCROSE (three-letter code: SUC) (formula: C₁₂H₂₂O₁₁).



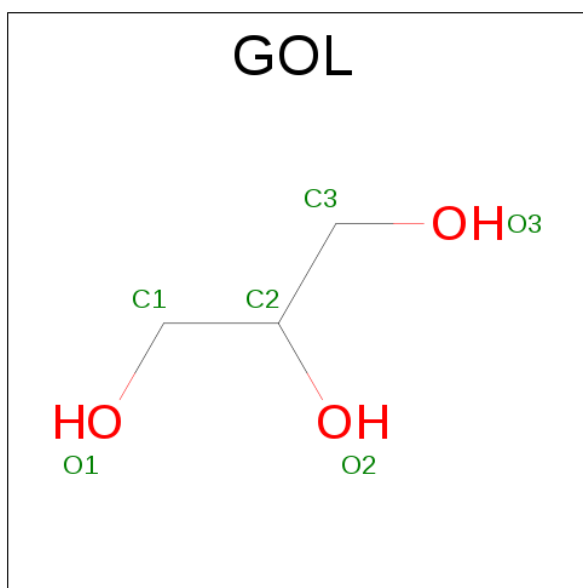
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			23	12	11		

- Molecule 5 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSE (three-letter code: CM5) (formula: $C_{23}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C		0	0
			6	6			
5	E	1	Total	C	O	0	0
			12	11	1		

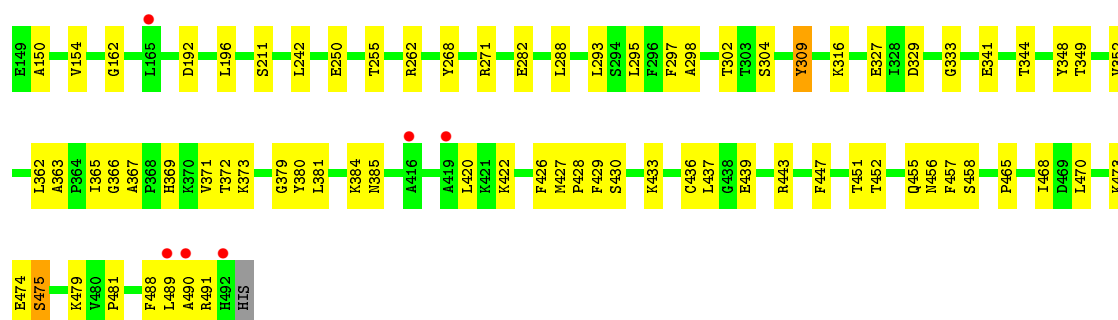
- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



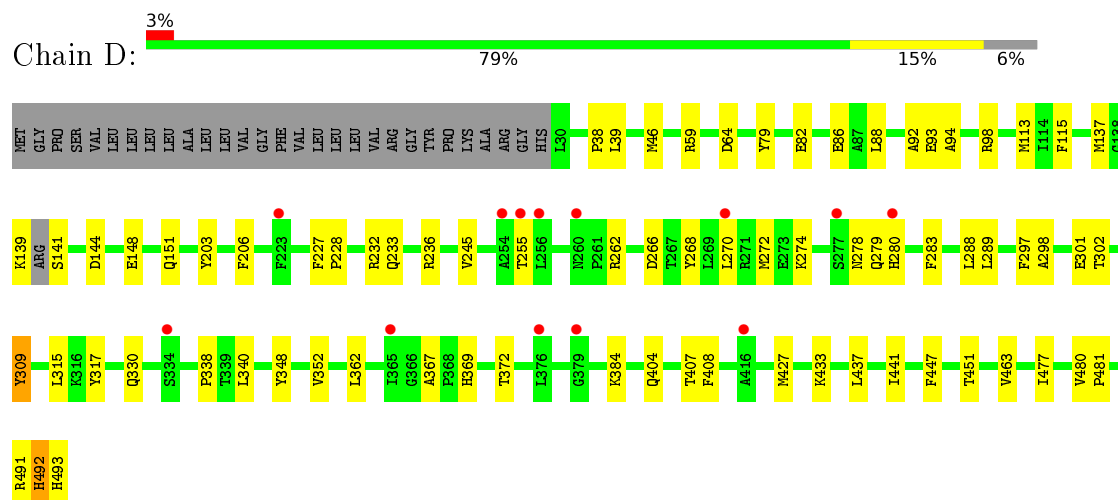
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

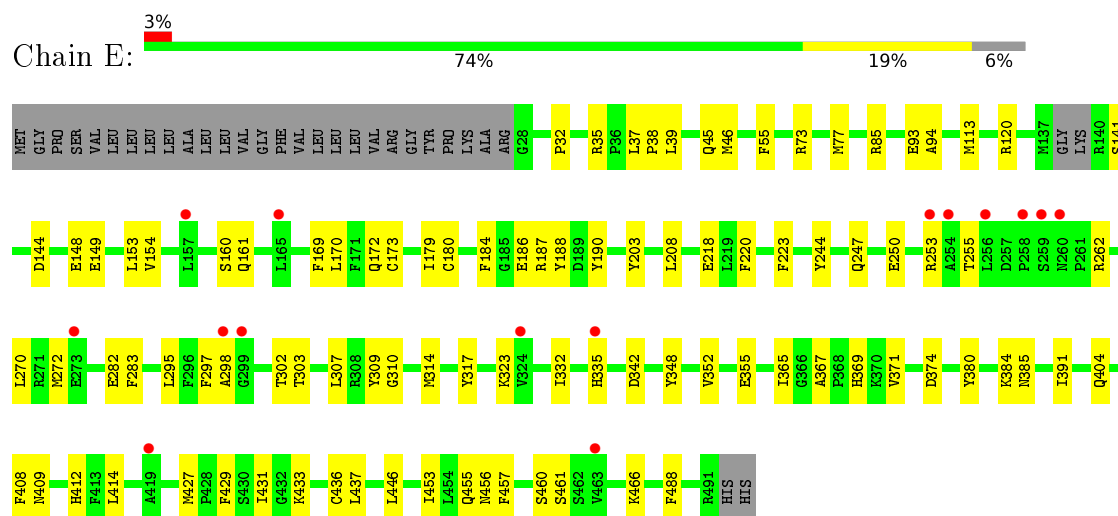
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	211	Total	O	0	0
			211	211		
7	B	59	Total	O	0	0
			59	59		
7	C	124	Total	O	0	0
			124	124		
7	D	106	Total	O	0	0
			106	106		
7	E	99	Total	O	0	0
			99	99		
7	F	60	Total	O	0	0
			60	60		



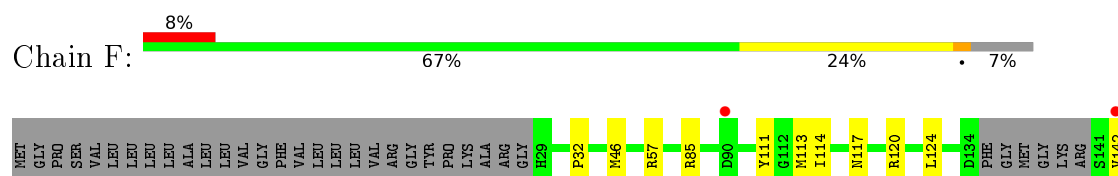
• Molecule 1: Cytochrome P450 family 2 subfamily B



• Molecule 1: Cytochrome P450 family 2 subfamily B



• Molecule 1: Cytochrome P450 family 2 subfamily B





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	98.08Å 106.07Å 106.20Å 64.61° 82.53° 69.93°	Depositor
Resolution (Å)	40.00 – 2.40 39.72 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.9 (40.00-2.40) 81.0 (39.72-2.40)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.216 , 0.283 0.229 , 0.277	Depositor DCC
R_{free} test set	6567 reflections (5.13%)	DCC
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 134688 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23024	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: GOL, CPZ, SUC, CM5, 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	0.57	0/3819	0.67	0/5163
1	B	0.61	0/3692	0.67	0/5008
1	C	0.57	0/3778	0.67	0/5114
1	D	0.56	0/3757	0.64	0/5090
1	E	0.51	0/3752	0.64	0/5080
1	F	0.60	0/3637	0.72	0/4936
All	All	0.57	0/22435	0.67	0/30391

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3727	0	3708	49	0
1	B	3602	0	3500	96	1
1	C	3685	0	3625	94	0
1	D	3665	0	3594	77	0
1	E	3661	0	3581	91	1
1	F	3558	0	3406	134	0
2	A	43	0	30	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	30	9	0
2	C	43	0	30	7	0
2	D	43	0	30	2	0
2	E	43	0	30	8	0
2	F	43	0	30	7	0
3	A	24	0	14	4	0
3	B	24	0	14	9	0
3	C	24	0	14	6	0
3	D	24	0	14	5	0
3	E	24	0	14	8	0
3	F	24	0	14	10	0
4	A	23	0	19	14	0
5	A	6	0	10	0	0
5	E	12	0	21	2	0
6	A	6	0	8	0	0
6	B	6	0	8	1	0
6	C	6	0	8	0	0
6	E	6	0	8	0	0
7	A	211	0	0	12	0
7	B	59	0	0	8	0
7	C	124	0	0	13	0
7	D	106	0	0	13	0
7	E	99	0	0	14	0
7	F	60	0	0	16	0
All	All	23024	0	21760	572	1

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 13.

The worst 5 of 572 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:E:455:GLN:NE2	7:E:601:HOH:O	1.79	1.15
4:A:504:SUC:O3'	4:A:504:SUC:O2	1.70	1.06
1:A:297:PHE:O	1:A:298:ALA:HB3	1.60	1.02
1:B:297:PHE:O	1:B:298:ALA:HB3	1.60	1.01
1:F:157:LEU:O	1:F:160:SER:HB3	1.62	1.00

All (1) 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:B:280:HIS:O	1:E:335:HIS:NE2[1_554]	2.03	0.17

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	462/493 (94%)	447 (97%)	15 (3%)	0	100	100
1	B	454/493 (92%)	432 (95%)	22 (5%)	0	100	100
1	C	463/493 (94%)	450 (97%)	12 (3%)	1 (0%)	52	69
1	D	459/493 (93%)	446 (97%)	12 (3%)	1 (0%)	52	69
1	E	458/493 (93%)	444 (97%)	14 (3%)	0	100	100
1	F	455/493 (92%)	424 (93%)	26 (6%)	5 (1%)	17	25
All	All	2751/2958 (93%)	2643 (96%)	101 (4%)	7 (0%)	46	63

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	475	SER
1	F	163	ALA
1	F	144	ASP
1	F	235	THR
1	D	492	HIS

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	408/433 (94%)	407 (100%)	1 (0%)	95	99
1	B	384/433 (89%)	383 (100%)	1 (0%)	94	98
1	C	396/433 (92%)	394 (100%)	2 (0%)	92	97
1	D	395/433 (91%)	393 (100%)	2 (0%)	92	97
1	E	393/433 (91%)	392 (100%)	1 (0%)	94	98
1	F	370/433 (86%)	365 (99%)	5 (1%)	74	88
All	All	2346/2598 (90%)	2334 (100%)	12 (0%)	92	97

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	309	TYR
1	E	309	TYR
1	F	268	TYR
1	D	113	MET
1	F	165	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	325	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 ⓘ

25 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	HEM	A	501	1,3	24,50,50	2.78	8 (33%)	16,82,82	1.43	2 (12%)
3	CPZ	A	502	2	11,13,13	0.49	0	13,17,17	0.88	0
3	CPZ	A	503	-	11,13,13	0.48	0	13,17,17	0.88	0
4	SUC	A	504	-	24,24,24	1.87	8 (33%)	36,36,36	1.92	12 (33%)
5	CM5	A	505	-	6,6,36	0.37	0	6,6,49	0.60	0
6	GOL	A	506	-	5,5,5	0.53	0	5,5,5	0.98	0
2	HEM	B	501	1,3	24,50,50	2.29	7 (29%)	16,82,82	1.86	5 (31%)
3	CPZ	B	502	2	11,13,13	0.75	0	13,17,17	1.28	1 (7%)
3	CPZ	B	503	-	11,13,13	0.58	0	13,17,17	1.29	2 (15%)
6	GOL	B	504	-	5,5,5	0.46	0	5,5,5	0.77	0
2	HEM	C	501	1,3	24,50,50	2.56	9 (37%)	16,82,82	1.65	2 (12%)
3	CPZ	C	502	2	11,13,13	0.49	0	13,17,17	0.88	0
3	CPZ	C	503	-	11,13,13	0.49	0	13,17,17	0.88	0
6	GOL	C	504	-	5,5,5	0.36	0	5,5,5	0.65	0
2	HEM	D	501	1,3	24,50,50	2.41	8 (33%)	16,82,82	1.81	5 (31%)
3	CPZ	D	502	-	11,13,13	0.50	0	13,17,17	0.88	0
3	CPZ	D	503	2	11,13,13	0.47	0	13,17,17	0.86	0
2	HEM	E	501	1,3	24,50,50	2.53	8 (33%)	16,82,82	1.91	4 (25%)
3	CPZ	E	502	2	11,13,13	0.49	0	13,17,17	0.88	0
3	CPZ	E	503	-	11,13,13	0.48	0	13,17,17	0.88	0
5	CM5	E	504	-	12,12,36	1.13	0	13,13,49	1.21	1 (7%)
6	GOL	E	505	-	5,5,5	0.42	0	5,5,5	0.60	0
2	HEM	F	501	3	24,50,50	2.56	7 (29%)	16,82,82	2.33	7 (43%)
3	CPZ	F	502	2	11,13,13	0.49	0	13,17,17	0.88	0
3	CPZ	F	503	-	11,13,13	0.49	0	13,17,17	0.88	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
2	HEM	A	501	1,3	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CPZ	A	502	2	-	0/4/4/4	0/2/2/2
3	CPZ	A	503	-	-	0/4/4/4	0/2/2/2
4	SUC	A	504	-	-	0/12/51/51	0/2/2/2
5	CM5	A	505	-	-	0/0/6/65	0/1/1/3
6	GOL	A	506	-	-	0/4/4/4	0/0/0/0
2	HEM	B	501	1,3	-	0/6/54/54	0/0/8/8
3	CPZ	B	502	2	-	0/4/4/4	0/2/2/2
3	CPZ	B	503	-	-	0/4/4/4	0/2/2/2
6	GOL	B	504	-	-	0/4/4/4	0/0/0/0
2	HEM	C	501	1,3	-	0/6/54/54	0/0/8/8
3	CPZ	C	502	2	-	0/4/4/4	0/2/2/2
3	CPZ	C	503	-	-	0/4/4/4	0/2/2/2
6	GOL	C	504	-	-	0/4/4/4	0/0/0/0
2	HEM	D	501	1,3	-	0/6/54/54	0/0/8/8
3	CPZ	D	502	-	-	0/4/4/4	0/2/2/2
3	CPZ	D	503	2	-	0/4/4/4	0/2/2/2
2	HEM	E	501	1,3	-	0/6/54/54	0/0/8/8
3	CPZ	E	502	2	-	0/4/4/4	0/2/2/2
3	CPZ	E	503	-	-	0/4/4/4	0/2/2/2
5	CM5	E	504	-	-	0/6/14/65	0/1/1/3
6	GOL	E	505	-	-	0/4/4/4	0/0/0/0
2	HEM	F	501	3	-	0/6/54/54	0/0/8/8
3	CPZ	F	502	2	-	0/4/4/4	0/2/2/2
3	CPZ	F	503	-	-	0/4/4/4	0/2/2/2

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3B-C2B	-8.92	1.29	1.40
2	A	501	HEM	C3C-C2C	-6.60	1.32	1.40
2	C	501	HEM	C3C-C2C	-6.60	1.32	1.40
2	F	501	HEM	C3B-C2B	-6.22	1.32	1.40
2	F	501	HEM	C3C-C2C	-6.08	1.32	1.40

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	SUC	O5-C1-C2	-5.44	98.98	110.28
2	E	501	HEM	C3C-CAC-CBC	-4.75	116.84	126.40
2	F	501	HEM	CAD-CBD-CGD	-4.68	103.67	112.78
4	A	504	SUC	O4-C4-C3	-4.57	100.06	110.36
2	F	501	HEM	C3C-CAC-CBC	-4.48	117.38	126.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 92 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	9	0
3	A	502	CPZ	4	0
3	A	503	CPZ	1	0
4	A	504	SUC	14	0
2	B	501	HEM	9	0
3	B	502	CPZ	5	0
3	B	503	CPZ	5	0
6	B	504	GOL	1	0
2	C	501	HEM	7	0
3	C	502	CPZ	4	0
3	C	503	CPZ	3	0
2	D	501	HEM	2	0
3	D	502	CPZ	4	0
3	D	503	CPZ	2	0
2	E	501	HEM	8	0
3	E	502	CPZ	6	0
3	E	503	CPZ	3	0
5	E	504	CM5	2	0
2	F	501	HEM	7	0
3	F	502	CPZ	5	0
3	F	503	CPZ	6	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	464/493 (94%)	-0.20	11 (2%) 62 61	19, 35, 60, 90	0
1	B	458/493 (92%)	0.14	25 (5%) 29 29	30, 50, 73, 86	0
1	C	465/493 (94%)	-0.16	6 (1%) 79 79	22, 43, 71, 90	0
1	D	463/493 (93%)	-0.09	13 (2%) 56 55	24, 45, 63, 84	0
1	E	462/493 (93%)	-0.03	15 (3%) 51 51	27, 48, 71, 79	0
1	F	458/493 (92%)	0.40	40 (8%) 13 12	27, 57, 75, 95	0
All	All	2770/2958 (93%)	0.01	110 (3%) 42 43	19, 47, 71, 95	0

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	492	HIS	5.2
1	F	490	ALA	5.2
1	F	259	SER	4.7
1	F	260	ASN	4.7
1	F	280	HIS	4.5

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 [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(Å ²)	Q<0.9
5	CM5	E	504	12/34	0.89	0.17	1.96	63,66,67,67	0
3	CPZ	D	502	12/12	0.84	0.22	1.40	57,58,61,65	0
3	CPZ	E	503	12/12	0.91	0.23	1.17	69,71,72,76	0
3	CPZ	B	503	12/12	0.87	0.26	0.92	68,70,74,76	0
3	CPZ	F	502	12/12	0.91	0.25	0.88	54,65,69,72	0
6	GOL	B	504	6/6	0.83	0.15	0.41	54,59,60,61	0
3	CPZ	A	503	12/12	0.86	0.22	0.31	49,52,56,60	0
3	CPZ	F	503	12/12	0.88	0.22	0.29	68,69,71,71	0
2	HEM	E	501	43/43	0.96	0.19	0.29	33,38,42,47	0
3	CPZ	E	502	12/12	0.95	0.21	0.26	42,46,46,47	0
2	HEM	B	501	43/43	0.97	0.20	-0.06	29,35,37,39	0
5	CM5	A	505	6/34	0.92	0.16	-0.17	55,55,56,56	0
3	CPZ	A	502	12/12	0.97	0.18	-0.18	31,33,35,37	0
2	HEM	A	501	43/43	0.98	0.21	-0.18	12,17,21,26	0
3	CPZ	B	502	12/12	0.96	0.20	-0.33	39,41,43,44	0
4	SUC	A	504	23/23	0.77	0.18	-0.34	35,54,62,63	0
3	CPZ	D	503	12/12	0.95	0.17	-0.36	35,42,49,52	0
3	CPZ	C	502	12/12	0.97	0.18	-0.37	40,42,44,45	0
2	HEM	C	501	43/43	0.98	0.16	-0.38	16,24,29,37	0
2	HEM	F	501	43/43	0.97	0.18	-0.42	40,44,49,53	0
2	HEM	D	501	43/43	0.97	0.17	-0.48	23,30,34,39	0
6	GOL	E	505	6/6	0.84	0.13	-0.80	65,67,68,69	0
3	CPZ	C	503	12/12	0.94	0.16	-1.18	49,51,53,60	0
6	GOL	C	504	6/6	0.76	0.14	-	65,69,69,71	0
6	GOL	A	506	6/6	0.74	0.10	-	47,52,53,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.