



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:28 PM UTC

PDB ID : 1CCL / pdb_00001ccl
Title : PROBING THE STRENGTH AND CHARACTER OF AN ASP-HIS-X HYDROGEN BOND BY INTRODUCING BURIED CHARGES
Authors : Cao, Y.; Goodin, D.B.; Mcree, D.E.
Deposited on : 1998-01-02
Resolution : 2.00 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

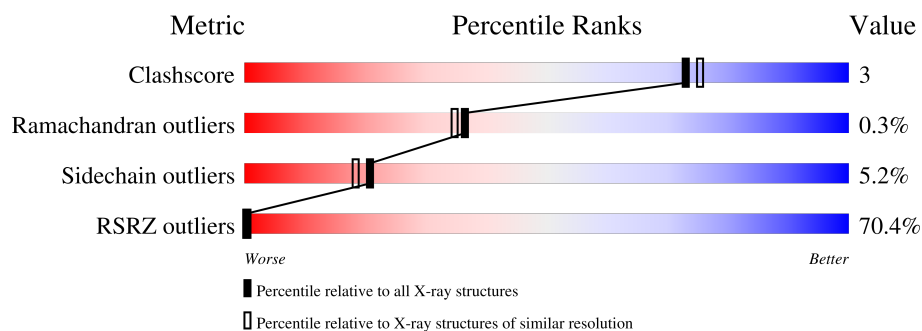
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	291	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3013 atoms, of which 515 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 C PEROXIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	291	Total	C	H	N	O	S	0	0	0
			2863	1498	515	393	451	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ILE	THR	engineered mutation	UNP P00431
A	152	GLY	ASP	engineered mutation	UNP P00431
A	202	LYS	PHE	engineered mutation	UNP P00431

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



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

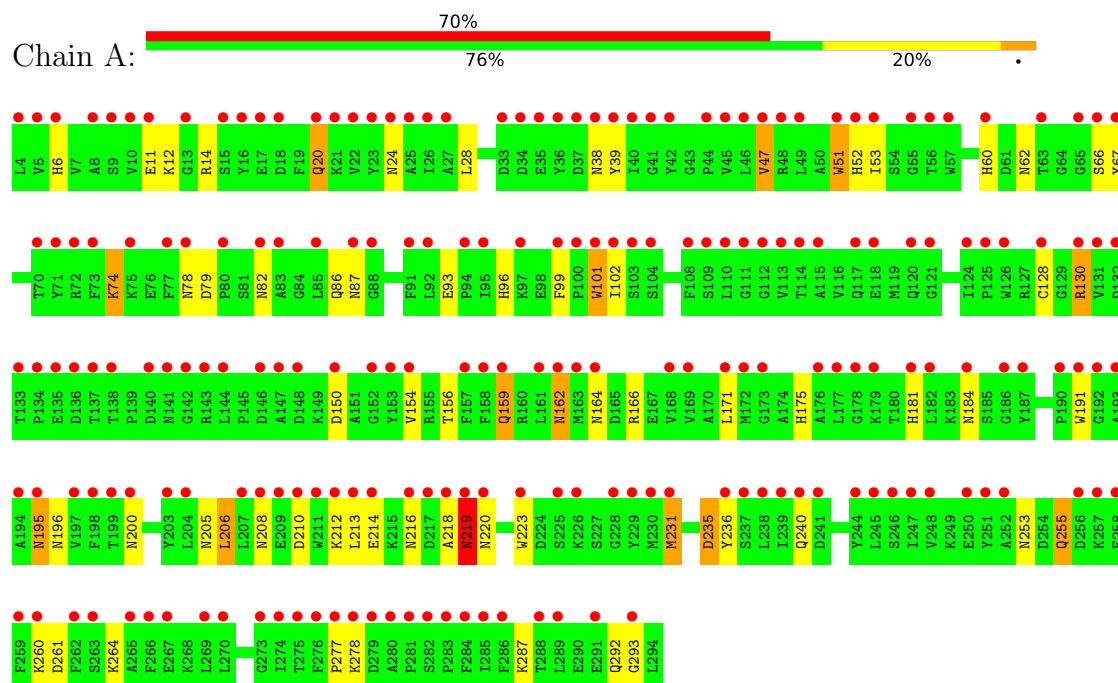
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total 107	O 107	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: CYTOCHROME C PEROXIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.40Å 73.20Å 44.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.00 5.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.00-2.00) 75.2 (5.00-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 1.99Å)	Xtriage
Refinement program	XTALVIEW, X-PLOR 3.1	Depositor
R, R_{free}	0.184 , (Not available) 0.502 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.61 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.55	EDS
Total number of atoms	3013	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.05% 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: 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	0.99	8/2413 (0.3%)	1.84	64/3265 (2.0%)

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	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	HIS	CD2-NE2	-7.06	1.30	1.37
1	A	60	HIS	CD2-NE2	-6.74	1.30	1.37
1	A	102	ILE	CA-CB	6.43	1.61	1.54
1	A	6	HIS	CD2-NE2	-6.36	1.30	1.37
1	A	52	HIS	CD2-NE2	-6.29	1.30	1.37
1	A	47	VAL	CA-CB	6.23	1.63	1.54
1	A	181	HIS	CD2-NE2	-5.19	1.32	1.37
1	A	175	HIS	CD2-NE2	-5.02	1.32	1.37

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	GLN	OE1-CD-NE2	-10.96	111.64	122.60
1	A	195	ASN	OD1-CG-ND2	-10.30	112.30	122.60
1	A	208	ASN	OD1-CG-ND2	-10.00	112.60	122.60
1	A	62	ASN	OD1-CG-ND2	-9.51	113.09	122.60
1	A	220	ASN	OD1-CG-ND2	-9.07	113.53	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	ASN	OD1-CG-ND2	-8.79	113.81	122.60
1	A	78	ASN	OD1-CG-ND2	-8.72	113.88	122.60
1	A	82	ASN	OD1-CG-ND2	-8.44	114.16	122.60
1	A	162	ASN	CA-CB-CG	8.40	121.00	112.60
1	A	195	ASN	N-CA-C	8.40	123.15	113.15
1	A	164	ASN	OD1-CG-ND2	-8.12	114.48	122.60
1	A	255	GLN	OE1-CD-NE2	-7.91	114.69	122.60
1	A	205	ASN	OD1-CG-ND2	-7.88	114.72	122.60
1	A	87	ASN	OD1-CG-ND2	-7.83	114.77	122.60
1	A	240	GLN	OE1-CD-NE2	-7.70	114.90	122.60
1	A	86	GLN	OE1-CD-NE2	-7.64	114.96	122.60
1	A	159	GLN	OE1-CD-NE2	-7.54	115.06	122.60
1	A	24	ASN	OD1-CG-ND2	-7.04	115.56	122.60
1	A	67	TYR	N-CA-C	7.00	119.51	111.11
1	A	219	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	A	195	ASN	CB-CG-ND2	6.98	126.88	116.40
1	A	292	GLN	OE1-CD-NE2	-6.85	115.75	122.60
1	A	79	ASP	CA-CB-CG	6.83	119.44	112.60
1	A	162	ASN	CA-C-O	6.80	130.23	120.51
1	A	278	LYS	CA-CB-CG	-6.79	100.51	114.10
1	A	210	ASP	CA-CB-CG	6.75	119.35	112.60
1	A	62	ASN	CB-CG-ND2	6.75	126.52	116.40
1	A	156	THR	CA-CB-OG1	-6.63	99.66	109.60
1	A	38	ASN	OD1-CG-ND2	-6.62	115.98	122.60
1	A	150	ASP	N-CA-C	6.50	119.32	109.95
1	A	277	PRO	CA-C-O	-6.31	114.00	122.08
1	A	253	ASN	CB-CG-ND2	6.28	125.81	116.40
1	A	208	ASN	CB-CG-ND2	6.05	125.48	116.40
1	A	162	ASN	N-CA-C	6.00	123.59	110.80
1	A	130	ARG	CG-CD-NE	-5.99	98.83	112.00
1	A	78	ASN	CB-CG-ND2	5.96	125.34	116.40
1	A	60	HIS	CB-CG-CD2	-5.92	123.51	131.20
1	A	219	ASN	CB-CG-ND2	5.87	125.20	116.40
1	A	66	SER	N-CA-C	5.86	119.68	112.54
1	A	216	ASN	OD1-CG-ND2	-5.79	116.81	122.60
1	A	52	HIS	CB-CG-CD2	-5.78	123.68	131.20
1	A	191	TRP	CB-CG-CD1	-5.65	118.43	126.90
1	A	195	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	154	VAL	N-CA-C	5.59	115.79	110.42
1	A	240	GLN	CG-CD-NE2	5.52	124.68	116.40
1	A	156	THR	CA-CB-CG2	5.52	119.88	110.50
1	A	128	CYS	O-C-N	-5.45	116.31	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	TRP	CB-CG-CD1	-5.42	118.77	126.90
1	A	101	TRP	CG-CD2-CE3	5.39	139.29	133.90
1	A	164	ASN	CB-CG-ND2	5.37	124.45	116.40
1	A	20	GLN	CG-CD-NE2	5.30	124.36	116.40
1	A	235	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	164	ASN	CA-CB-CG	5.25	117.85	112.60
1	A	184	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	A	220	ASN	CB-CG-ND2	5.15	124.12	116.40
1	A	93	GLU	CA-C-N	5.15	124.94	119.28
1	A	93	GLU	C-N-CA	5.15	124.94	119.28
1	A	181	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	A	196	ASN	CA-C-O	5.13	125.55	120.32
1	A	51	TRP	CG-CD2-CE3	5.09	138.99	133.90
1	A	82	ASN	CB-CG-ND2	5.08	124.03	116.40
1	A	99	PHE	CA-C-N	5.05	124.71	119.56
1	A	99	PHE	C-N-CA	5.05	124.71	119.56
1	A	277	PRO	O-C-N	-5.02	116.88	123.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39	TYR	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	2348	515	2232	15	45
2	A	43	0	30	0	0
3	A	107	0	0	2	12
All	All	2498	515	2262	15	45

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 3.

All (15) 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:231:MET:HE1	1:A:236:TYR:HD1	1.46	0.80
1:A:20:GLN:HE22	1:A:287:LYS:H	1.40	0.69
1:A:231:MET:HE1	1:A:236:TYR:CD1	2.29	0.65
1:A:74:LYS:HD2	1:A:74:LYS:H	1.67	0.58
1:A:200:ASN:H	1:A:255:GLN:HE21	1.51	0.56
1:A:20:GLN:HE22	1:A:287:LYS:N	2.04	0.54
1:A:223:TRP:HB2	1:A:231:MET:HE2	1.91	0.53
1:A:231:MET:HG2	1:A:235:ASP:HB2	1.91	0.51
1:A:130:ARG:NE	3:A:326:HOH:O	2.47	0.48
1:A:20:GLN:NE2	1:A:287:LYS:H	2.10	0.47
1:A:206:LEU:HD12	1:A:231:MET:SD	2.56	0.45
1:A:130:ARG:CZ	3:A:326:HOH:O	2.65	0.43
1:A:231:MET:HG2	1:A:235:ASP:CB	2.50	0.41
1:A:74:LYS:H	1:A:74:LYS:CD	2.33	0.41
1:A:218:ALA:O	1:A:219:ASN:HB2	2.21	0.41

All (45) 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:14:ARG:NH2	1:A:213:LEU:C[4_5610]	0.42	1.78
1:A:12:LYS:CA	1:A:214:GLU:OE2[4_5610]	0.83	1.37
1:A:14:ARG:CZ	1:A:213:LEU:O[4_5610]	0.83	1.37
1:A:14:ARG:NE	1:A:213:LEU:O[4_5610]	0.94	1.26
1:A:14:ARG:CZ	1:A:213:LEU:C[4_5610]	1.07	1.13
1:A:14:ARG:NH2	1:A:213:LEU:CA[4_5610]	1.11	1.09
1:A:212:LYS:CG	3:A:372:HOH:O[4_4610]	1.15	1.05
1:A:12:LYS:C	1:A:214:GLU:OE2[4_5610]	1.33	0.87
1:A:212:LYS:CD	3:A:372:HOH:O[4_4610]	1.33	0.87
1:A:264:LYS:HZ3	3:A:389:HOH:O[3_559]	0.73	0.87
1:A:212:LYS:CB	3:A:372:HOH:O[4_4610]	1.34	0.86
1:A:14:ARG:HH22	1:A:213:LEU:CA[4_5610]	0.77	0.83
1:A:212:LYS:NZ	3:A:374:HOH:O[4_4610]	1.37	0.83
1:A:12:LYS:O	1:A:214:GLU:CG[4_5610]	1.38	0.82
1:A:12:LYS:N	1:A:214:GLU:OE2[4_5610]	1.40	0.80
1:A:14:ARG:NH2	1:A:213:LEU:O[4_5610]	1.41	0.79
1:A:12:LYS:O	1:A:214:GLU:CB[4_5610]	1.43	0.77
1:A:264:LYS:NZ	3:A:389:HOH:O[3_559]	1.46	0.74
1:A:12:LYS:O	1:A:214:GLU:CD[4_5610]	1.49	0.71
1:A:212:LYS:CE	3:A:374:HOH:O[4_4610]	1.53	0.67
1:A:214:GLU:CG	3:A:373:HOH:O[4_4610]	1.53	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ARG:NH2	1:A:214:GLU:N[4_5610]	1.62	0.58
1:A:261:ASP:OD1	3:A:389:HOH:O[3_559]	1.68	0.52
1:A:12:LYS:CB	1:A:214:GLU:OE1[4_5610]	1.72	0.48
1:A:12:LYS:C	1:A:214:GLU:CD[4_5610]	1.75	0.45
1:A:14:ARG:HH21	1:A:213:LEU:C[4_5610]	1.17	0.43
1:A:12:LYS:CB	1:A:214:GLU:OE2[4_5610]	1.80	0.40
1:A:11:GLU:CA	1:A:212:LYS:HZ1[4_5610]	1.22	0.38
1:A:14:ARG:CZ	1:A:214:GLU:N[4_5610]	1.83	0.37
1:A:101:TRP:CB	1:A:213:LEU:H[4_5610]	1.23	0.37
1:A:12:LYS:O	1:A:214:GLU:OE2[4_5610]	1.84	0.36
1:A:212:LYS:CE	3:A:372:HOH:O[4_4610]	1.84	0.36
1:A:14:ARG:HE	1:A:213:LEU:O[4_5610]	1.26	0.34
1:A:212:LYS:HZ3	3:A:374:HOH:O[4_4610]	1.26	0.34
1:A:14:ARG:HH22	1:A:213:LEU:C[4_5610]	1.27	0.33
1:A:12:LYS:CA	1:A:214:GLU:CD[4_5610]	1.89	0.31
1:A:101:TRP:CB	1:A:213:LEU:N[4_5610]	1.97	0.23
1:A:12:LYS:CB	1:A:214:GLU:CD[4_5610]	2.00	0.20
1:A:14:ARG:NE	1:A:213:LEU:C[4_5610]	2.01	0.19
1:A:293:GLY:O	3:A:331:HOH:O[3_549]	2.03	0.17
1:A:14:ARG:HH21	1:A:213:LEU:CA[4_5610]	1.47	0.13
1:A:14:ARG:NH2	1:A:213:LEU:N[4_5610]	2.08	0.12
1:A:14:ARG:NH1	1:A:213:LEU:O[4_5610]	2.10	0.10
1:A:14:ARG:NH1	1:A:213:LEU:C[4_5610]	2.13	0.07
1:A:14:ARG:NH2	1:A:213:LEU:CB[4_5610]	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	289/291 (99%)	279 (96%)	9 (3%)	1 (0%)	36	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	ASN

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	249/249 (100%)	236 (95%)	13 (5%)	21	18

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	47	VAL
1	A	51	TRP
1	A	53	ILE
1	A	74	LYS
1	A	159	GLN
1	A	166	ARG
1	A	171	LEU
1	A	195	ASN
1	A	206	LEU
1	A	219	ASN
1	A	231	MET
1	A	260	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	20	GLN
1	A	24	ASN
1	A	87	ASN
1	A	255	GLN
1	A	292	GLN

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](#)

1 ligand is 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	1	3,1	50,50,50	2.23	23 (46%)	67,82,82	1.05	4 (5%)

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	1	3,1	-	4/14/54/54	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	HEM	FE-NB	4.43	2.08	1.94
2	A	1	HEM	FE-ND	4.14	2.07	1.94
2	A	1	HEM	C1B-NB	-3.79	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	HEM	C4D-ND	-3.62	1.34	1.40
2	A	1	HEM	FE-NA	3.48	2.06	1.95
2	A	1	HEM	C4D-C3D	-3.42	1.39	1.45
2	A	1	HEM	FE-NC	3.27	2.06	1.95
2	A	1	HEM	CBC-CAC	3.14	1.45	1.30
2	A	1	HEM	C3C-C4C	-3.14	1.40	1.46
2	A	1	HEM	C4C-NC	-3.13	1.33	1.39
2	A	1	HEM	C1A-C2A	-2.99	1.38	1.44
2	A	1	HEM	C4A-NA	-2.97	1.34	1.39
2	A	1	HEM	CBB-CAB	2.92	1.44	1.30
2	A	1	HEM	C1A-NA	-2.68	1.34	1.39
2	A	1	HEM	C1D-ND	-2.65	1.33	1.38
2	A	1	HEM	C1C-C2C	-2.62	1.40	1.45
2	A	1	HEM	C3B-C4B	-2.51	1.40	1.44
2	A	1	HEM	CAB-C3B	-2.46	1.40	1.47
2	A	1	HEM	C1D-C2D	-2.44	1.39	1.44
2	A	1	HEM	O2A-CGA	-2.31	1.23	1.30
2	A	1	HEM	CAC-C3C	-2.29	1.41	1.47
2	A	1	HEM	O2D-CGD	-2.23	1.23	1.30
2	A	1	HEM	C1C-NC	-2.07	1.35	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	HEM	C3C-C2C-C1C	-3.06	104.15	107.05
2	A	1	HEM	CMD-C2D-C1D	2.16	128.40	125.03
2	A	1	HEM	O2D-CGD-CBD	2.15	120.80	114.00
2	A	1	HEM	C4B-C3B-C2B	-2.09	105.36	107.28

There are no chirality outliers.

All (4) torsion outliers are listed below:

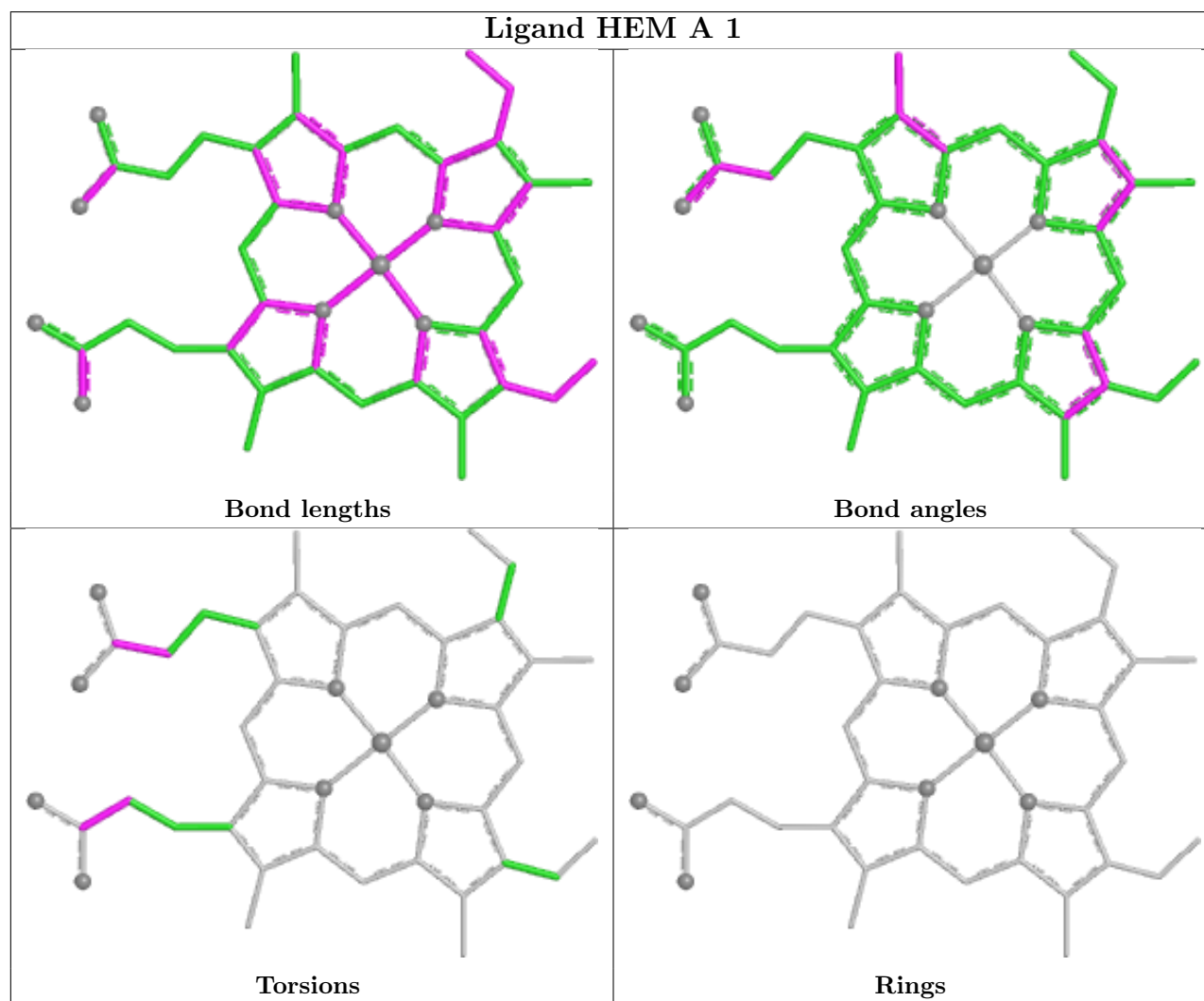
Mol	Chain	Res	Type	Atoms
2	A	1	HEM	CAA-CBA-CGA-O2A
2	A	1	HEM	CAA-CBA-CGA-O1A
2	A	1	HEM	CAD-CBD-CGD-O2D
2	A	1	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	291/291 (100%)	2.54	205 (70%) 0 0	10, 17, 29, 41	0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	251	TYR	6.0
1	A	192	GLY	6.0
1	A	193	ALA	5.3
1	A	5	VAL	5.2
1	A	219	ASN	5.0
1	A	27	ALA	5.0
1	A	187	TYR	4.9
1	A	236	TYR	4.9
1	A	35	GLU	4.8
1	A	204	LEU	4.8
1	A	282	SER	4.8
1	A	283	PRO	4.7
1	A	83	ALA	4.6
1	A	198	PHE	4.6
1	A	77	PHE	4.5
1	A	101	TRP	4.5
1	A	163	MET	4.3
1	A	51	TRP	4.3
1	A	223	TRP	4.3
1	A	195	ASN	4.2
1	A	276	PHE	4.2
1	A	110	LEU	4.2
1	A	40	ILE	4.2
1	A	275	THR	4.1
1	A	168	VAL	4.0
1	A	4	LEU	4.0
1	A	36	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	65	GLY	4.0
1	A	57	TRP	3.9
1	A	125	PRO	3.9
1	A	280	ALA	3.9
1	A	128	CYS	3.8
1	A	108	PHE	3.8
1	A	13	GLY	3.8
1	A	39	TYR	3.8
1	A	25	ALA	3.8
1	A	284	PHE	3.8
1	A	126	TRP	3.8
1	A	24	ASN	3.8
1	A	10	VAL	3.8
1	A	231	MET	3.8
1	A	49	LEU	3.7
1	A	94	PRO	3.7
1	A	131	VAL	3.7
1	A	259	PHE	3.7
1	A	269	LEU	3.7
1	A	67	TYR	3.7
1	A	286	PHE	3.6
1	A	71	TYR	3.6
1	A	247	ILE	3.6
1	A	92	LEU	3.6
1	A	16	TYR	3.6
1	A	194	ALA	3.5
1	A	240	GLN	3.5
1	A	22	VAL	3.5
1	A	293	GLY	3.5
1	A	33	ASP	3.4
1	A	230	MET	3.4
1	A	208	ASN	3.4
1	A	220	ASN	3.4
1	A	85	LEU	3.4
1	A	73	PHE	3.4
1	A	120	GLN	3.4
1	A	109	SER	3.3
1	A	95	ILE	3.3
1	A	115	ALA	3.3
1	A	38	ASN	3.3
1	A	56	THR	3.3
1	A	75	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	241	ASP	3.3
1	A	63	THR	3.2
1	A	143	ARG	3.2
1	A	99	PHE	3.2
1	A	142	GLY	3.2
1	A	211	TRP	3.2
1	A	72	ARG	3.2
1	A	144	LEU	3.2
1	A	270	LEU	3.2
1	A	274	ILE	3.2
1	A	191	TRP	3.1
1	A	34	ASP	3.1
1	A	111	GLY	3.1
1	A	173	GLY	3.1
1	A	171	LEU	3.1
1	A	258	PHE	3.1
1	A	132	ASP	3.1
1	A	141	ASN	3.1
1	A	213	LEU	3.1
1	A	184	ASN	3.0
1	A	182	LEU	3.0
1	A	200	ASN	2.9
1	A	186	GLY	2.9
1	A	8	ALA	2.9
1	A	252	ALA	2.9
1	A	135	GLU	2.9
1	A	9	SER	2.9
1	A	136	ASP	2.9
1	A	181	HIS	2.9
1	A	154	VAL	2.9
1	A	100	PRO	2.9
1	A	17	GLU	2.8
1	A	158	PHE	2.8
1	A	229	TYR	2.8
1	A	152	GLY	2.8
1	A	177	LEU	2.8
1	A	103	SER	2.8
1	A	23	TYR	2.8
1	A	53	ILE	2.8
1	A	102	ILE	2.8
1	A	285	ILE	2.8
1	A	262	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	244	TYR	2.8
1	A	265	ALA	2.8
1	A	239	ILE	2.8
1	A	11	GLU	2.7
1	A	210	ASP	2.7
1	A	238	LEU	2.7
1	A	281	PRO	2.7
1	A	203	TYR	2.7
1	A	80	PRO	2.7
1	A	250	GLU	2.7
1	A	37	ASP	2.7
1	A	70	THR	2.7
1	A	134	PRO	2.7
1	A	267	GLU	2.7
1	A	257	LYS	2.7
1	A	46	LEU	2.6
1	A	148	ASP	2.6
1	A	217	ASP	2.6
1	A	138	THR	2.6
1	A	266	PHE	2.5
1	A	291	GLU	2.5
1	A	133	THR	2.5
1	A	279	ASP	2.5
1	A	147	ALA	2.5
1	A	237	SER	2.5
1	A	207	LEU	2.5
1	A	118	GLU	2.5
1	A	197	VAL	2.5
1	A	60	HIS	2.5
1	A	78	ASN	2.5
1	A	150	ASP	2.5
1	A	218	ALA	2.5
1	A	273	GLY	2.5
1	A	42	TYR	2.5
1	A	121	GLY	2.5
1	A	216	ASN	2.5
1	A	15	SER	2.4
1	A	246	SER	2.4
1	A	288	THR	2.4
1	A	159	GLN	2.4
1	A	47	VAL	2.4
1	A	140	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	161	LEU	2.4
1	A	190	PRO	2.4
1	A	21	LYS	2.4
1	A	88	GLY	2.3
1	A	91	PHE	2.3
1	A	169	VAL	2.3
1	A	214	GLU	2.3
1	A	153	TYR	2.3
1	A	162	ASN	2.3
1	A	112	GLY	2.3
1	A	245	LEU	2.3
1	A	256	ASP	2.3
1	A	130	ARG	2.3
1	A	212	LYS	2.3
1	A	104	SER	2.3
1	A	225	SER	2.3
1	A	226	LYS	2.3
1	A	278	LYS	2.3
1	A	289	LEU	2.3
1	A	157	PHE	2.2
1	A	45	VAL	2.2
1	A	124	ILE	2.2
1	A	137	THR	2.2
1	A	18	ASP	2.2
1	A	176	ALA	2.2
1	A	52	HIS	2.2
1	A	20	GLN	2.2
1	A	66	SER	2.2
1	A	44	PRO	2.1
1	A	146	ASP	2.2
1	A	113	VAL	2.1
1	A	48	ARG	2.1
1	A	26	ILE	2.1
1	A	87	ASN	2.1
1	A	117	GLN	2.1
1	A	277	PRO	2.1
1	A	55	GLY	2.1
1	A	228	GLY	2.1
1	A	260	LYS	2.1
1	A	263	SER	2.1
1	A	172	MET	2.1
1	A	199	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	97	LYS	2.1
1	A	209	GLU	2.0
1	A	82	ASN	2.0
1	A	164	ASN	2.0
1	A	6	HIS	2.0
1	A	179	LYS	2.0
1	A	178	GLY	2.0
1	A	248	VAL	2.0
1	A	114	THR	2.0
1	A	41	GLY	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

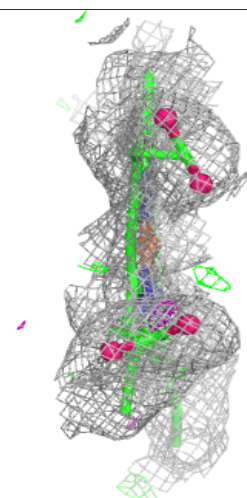
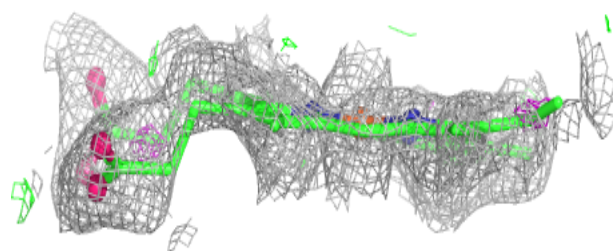
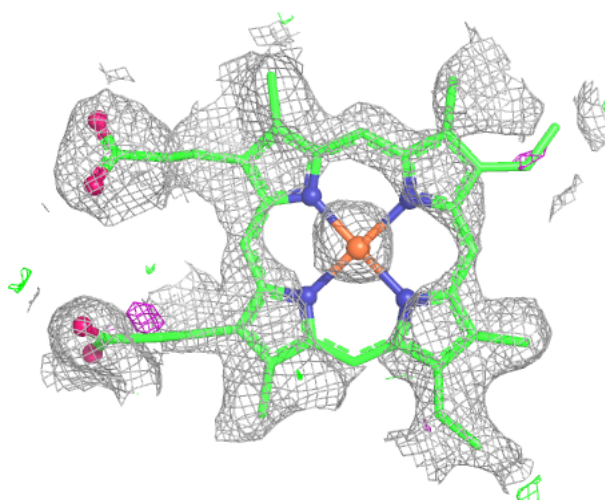
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	A	1	43/43	0.67	0.15	12,15,18,25	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 HEM A 1:

$2mF_o-DF_c$ (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.