



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 11:33 PM EDT

PDB ID : 1QPW / pdb_00001qpw
Title : CRYSTAL STRUCTURE DETERMINATION OF PORCINE
HEMOGLOBIN AT 1.8A RESOLUTION
Authors : Lu, T.-H.; Panneerselvam, K.; Liaw, Y.-C.; Kan, P.; Lee, C.-J.
Deposited on : 1999-05-30
Resolution : 1.80 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

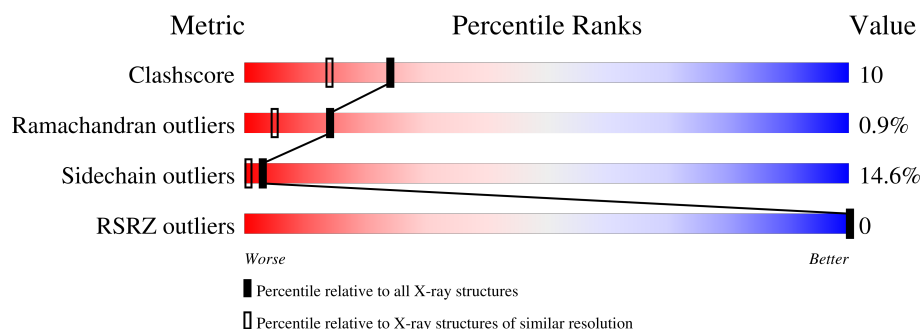
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	141	
1	C	141	
2	B	146	
2	D	146	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5148 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 PORCINE HEMOGLOBIN (ALPHA SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1064	677	192	193	2			
1	C	141	Total	C	N	O	S	0	0	0
			1064	677	192	193	2			

- Molecule 2 is a protein called PORCINE HEMOGLOBIN (BETA SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1135	726	203	204	2			
2	D	146	Total	C	N	O	S	0	0	0
			1135	726	203	204	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	125	ASP	ASN	conflict	UNP P01965
D	125	ASP	ASN	conflict	UNP P02067

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O	0	0
			2	2		
4	C	1	Total	O	0	0
			2	2		

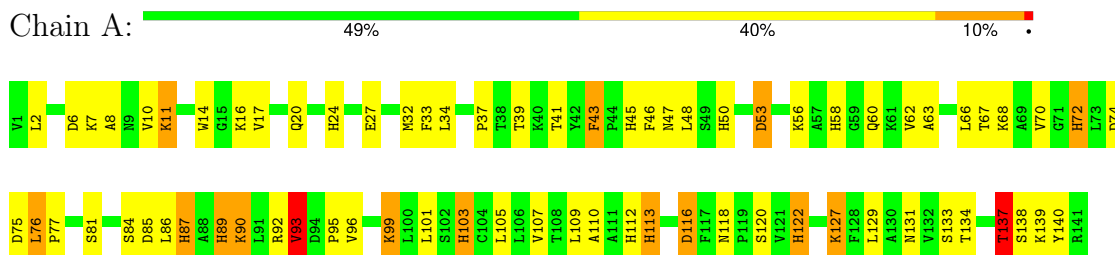
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	104	Total	O	0	0
			104	104		
5	B	143	Total	O	0	0
			143	143		
5	C	135	Total	O	0	0
			135	135		
5	D	192	Total	O	0	0
			192	192		

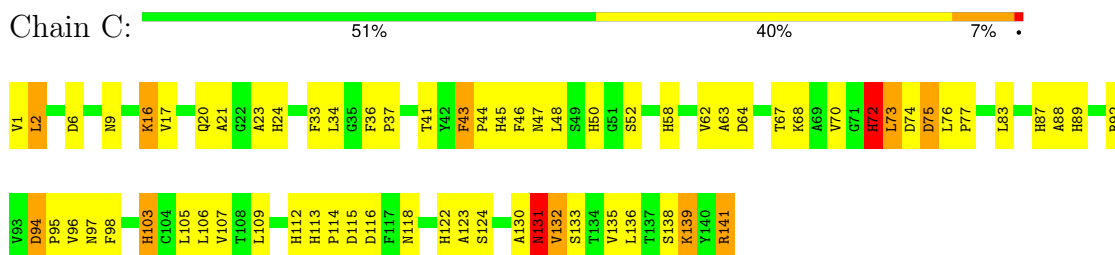
3 Residue-property plots [i](#)

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.

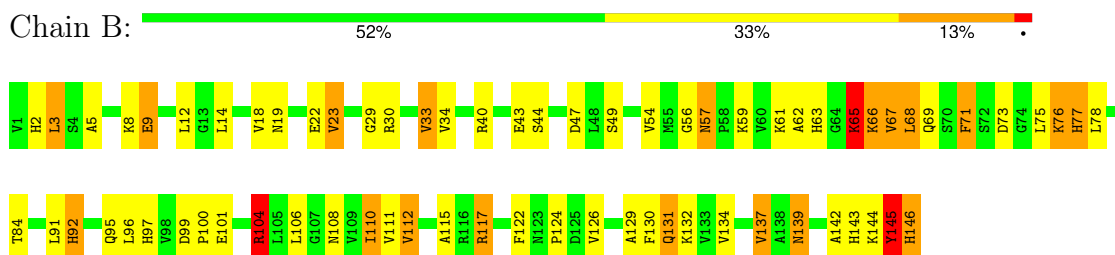
• Molecule 1: PORCINE HEMOGLOBIN (ALPHA SUBUNIT)



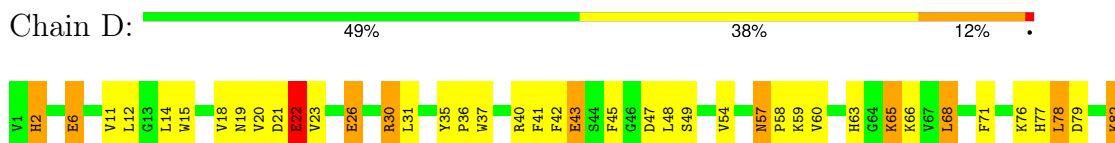
• Molecule 1: PORCINE HEMOGLOBIN (ALPHA SUBUNIT)



• Molecule 2: PORCINE HEMOGLOBIN (BETA SUBUNIT)



• Molecule 2: PORCINE HEMOGLOBIN (BETA SUBUNIT)





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.10Å 72.27Å 114.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.80 8.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (8.00-1.80) 69.3 (8.00-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.80Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.207 , 0.251 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 76.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5148	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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, OXY

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	1.49	14/1091 (1.3%)	2.29	54/1480 (3.6%)
1	C	1.57	15/1091 (1.4%)	2.24	60/1480 (4.1%)
2	B	1.41	11/1160 (0.9%)	2.15	49/1568 (3.1%)
2	D	1.42	7/1160 (0.6%)	2.24	67/1568 (4.3%)
All	All	1.47	47/4502 (1.0%)	2.23	230/6096 (3.8%)

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
2	D	0	1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	HIS	CD2-NE2	-12.51	1.24	1.37
2	D	92	HIS	CD2-NE2	-12.08	1.24	1.37
2	B	92	HIS	CD2-NE2	-10.71	1.26	1.37
1	A	87	HIS	CE1-NE2	-9.26	1.23	1.32
1	A	93	VAL	CA-CB	8.57	1.65	1.54
2	D	92	HIS	CE1-NE2	-7.87	1.24	1.32
1	A	87	HIS	CD2-NE2	-7.59	1.29	1.37
2	B	97	HIS	CD2-NE2	-7.15	1.29	1.37
1	C	87	HIS	CE1-NE2	-7.09	1.25	1.32
1	A	58	HIS	CD2-NE2	-7.02	1.30	1.37
1	A	72	HIS	CD2-NE2	-6.92	1.30	1.37
1	A	103	HIS	CD2-NE2	-6.83	1.30	1.37
1	C	45	HIS	CD2-NE2	-6.76	1.30	1.37
1	A	122	HIS	CD2-NE2	-6.52	1.30	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	63	HIS	CD2-NE2	-6.42	1.30	1.37
1	C	58	HIS	CD2-NE2	-6.34	1.30	1.37
2	B	112	VAL	CA-CB	6.14	1.62	1.54
1	C	50	HIS	CG-ND1	-6.11	1.31	1.38
2	D	77	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	112	HIS	CD2-NE2	-5.96	1.31	1.37
1	C	24	HIS	CD2-NE2	-5.94	1.31	1.37
1	A	45	HIS	CD2-NE2	-5.92	1.31	1.37
2	D	63	HIS	CD2-NE2	-5.87	1.31	1.37
1	A	87	HIS	CG-ND1	-5.85	1.31	1.38
2	B	54	VAL	CA-CB	5.85	1.60	1.54
1	C	113	HIS	CD2-NE2	-5.79	1.31	1.37
1	C	58	HIS	CG-ND1	-5.76	1.31	1.38
1	C	122	HIS	CD2-NE2	-5.76	1.31	1.37
1	A	89	HIS	CD2-NE2	-5.72	1.31	1.37
2	D	26	GLU	CA-CB	-5.70	1.43	1.53
2	B	67	VAL	CA-CB	5.68	1.62	1.54
2	B	23	VAL	CA-CB	5.68	1.62	1.54
1	C	62	VAL	CA-CB	5.63	1.61	1.54
1	C	50	HIS	CD2-NE2	-5.61	1.31	1.37
1	C	103	HIS	CD2-NE2	-5.55	1.31	1.37
1	A	24	HIS	CD2-NE2	-5.47	1.31	1.37
2	B	143	HIS	CD2-NE2	-5.45	1.31	1.37
2	D	97	HIS	CD2-NE2	-5.44	1.31	1.37
1	A	50	HIS	CD2-NE2	-5.44	1.31	1.37
2	B	2	HIS	CD2-NE2	-5.41	1.31	1.37
1	C	72	HIS	CD2-NE2	-5.41	1.31	1.37
1	A	112	HIS	CG-ND1	-5.40	1.32	1.38
2	B	77	HIS	CD2-NE2	-5.35	1.31	1.37
1	C	113	HIS	CG-ND1	-5.23	1.32	1.38
2	B	146	HIS	CG-ND1	-5.19	1.32	1.38
2	D	2	HIS	CD2-NE2	-5.19	1.32	1.37
1	C	107	VAL	CA-CB	-5.17	1.48	1.54

All (230) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	87	HIS	CE1-NE2-CD2	15.61	124.61	109.00
2	D	92	HIS	CE1-NE2-CD2	14.04	123.04	109.00
1	A	53	ASP	CA-CB-CG	12.38	124.98	112.60
1	C	97	ASN	OD1-CG-ND2	-9.88	112.72	122.60
1	C	9	ASN	OD1-CG-ND2	-9.59	113.01	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	87	HIS	ND1-CE1-NE2	-9.40	99.00	108.40
2	B	131	GLN	CG-CD-NE2	9.22	130.23	116.40
1	C	87	HIS	CG-CD2-NE2	-9.01	98.19	107.20
2	D	54	VAL	N-CA-C	-8.84	102.11	110.42
1	A	89	HIS	CA-CB-CG	8.79	122.59	113.80
1	A	131	ASN	OD1-CG-ND2	-8.73	113.87	122.60
2	B	47	ASP	CA-CB-CG	8.54	121.14	112.60
2	D	92	HIS	CA-CB-CG	-8.53	105.27	113.80
1	C	45	HIS	CB-CG-CD2	-8.42	120.25	131.20
2	D	21	ASP	CA-CB-CG	8.38	120.98	112.60
1	A	87	HIS	CE1-NE2-CD2	8.31	117.31	109.00
2	D	43	GLU	CA-CB-CG	8.10	130.30	114.10
1	C	45	HIS	CB-CG-ND1	8.09	134.84	122.70
2	B	9	GLU	CB-CG-CD	8.00	126.20	112.60
2	D	92	HIS	ND1-CE1-NE2	-8.00	100.40	108.40
2	B	92	HIS	CB-CG-CD2	-7.96	120.85	131.20
1	A	137	THR	N-CA-CB	-7.86	98.01	110.98
2	D	125	ASP	CA-CB-CG	-7.84	104.76	112.60
2	D	108	ASN	OD1-CG-ND2	-7.73	114.87	122.60
2	D	23	VAL	N-CA-C	7.69	117.80	110.42
2	D	92	HIS	CG-CD2-NE2	-7.69	99.51	107.20
2	B	108	ASN	OD1-CG-ND2	-7.68	114.92	122.60
1	C	114	PRO	CA-C-N	7.67	130.89	120.54
1	C	114	PRO	C-N-CA	7.67	130.89	120.54
1	C	118	ASN	N-CA-C	-7.58	101.42	110.13
1	A	27	GLU	CB-CG-CD	7.50	125.35	112.60
2	D	35	TYR	CA-C-N	7.44	128.10	119.47
2	D	35	TYR	C-N-CA	7.44	128.10	119.47
2	D	47	ASP	CA-CB-CG	7.32	119.92	112.60
2	B	92	HIS	CA-CB-CG	-7.30	106.50	113.80
1	A	46	PHE	CA-CB-CG	7.29	121.09	113.80
1	A	43	PHE	CA-CB-CG	-7.21	106.59	113.80
1	A	87	HIS	CA-C-O	-7.21	112.24	120.24
1	A	87	HIS	CG-CD2-NE2	-7.17	100.03	107.20
2	D	134	VAL	N-CA-C	-7.16	103.20	111.00
1	A	116	ASP	N-CA-CB	-7.16	100.70	111.15
2	D	57	ASN	CA-C-N	7.14	126.67	119.24
2	D	57	ASN	C-N-CA	7.14	126.67	119.24
1	C	87	HIS	N-CA-C	7.12	118.94	111.03
1	C	94	ASP	CA-CB-CG	7.12	119.72	112.60
2	B	92	HIS	CE1-NE2-CD2	7.06	116.06	109.00
2	B	131	GLN	OE1-CD-NE2	-6.93	115.67	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	VAL	N-CA-C	-6.91	104.12	110.82
2	B	77	HIS	CA-C-N	6.84	130.36	120.38
2	B	77	HIS	C-N-CA	6.84	130.36	120.38
2	D	18	VAL	O-C-N	-6.80	115.21	122.83
1	C	87	HIS	CB-CG-CD2	-6.77	122.40	131.20
2	B	19	ASN	OD1-CG-ND2	-6.74	115.86	122.60
2	D	2	HIS	CA-CB-CG	-6.73	107.07	113.80
2	D	83	GLY	CA-C-O	-6.71	113.84	120.75
2	B	76	LYS	CA-C-O	6.70	130.10	120.51
1	C	24	HIS	CA-CB-CG	-6.70	107.10	113.80
2	B	99	ASP	CA-C-N	6.69	126.38	119.56
2	B	99	ASP	C-N-CA	6.69	126.38	119.56
2	B	73	ASP	CA-CB-CG	6.68	119.28	112.60
2	D	122	PHE	CA-CB-CG	-6.68	107.12	113.80
1	C	131	ASN	CA-CB-CG	6.64	119.24	112.60
2	D	49	SER	N-CA-C	6.63	122.52	113.37
2	D	127	GLN	OE1-CD-NE2	-6.63	115.97	122.60
1	A	122	HIS	CB-CG-CD2	-6.58	122.65	131.20
2	B	97	HIS	CB-CG-CD2	-6.58	122.65	131.20
1	A	85	ASP	CA-CB-CG	6.56	119.16	112.60
1	C	112	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	C	94	ASP	CA-C-N	6.55	128.03	119.84
1	C	94	ASP	C-N-CA	6.55	128.03	119.84
1	C	46	PHE	CA-CB-CG	6.54	120.33	113.80
1	C	75	ASP	CA-CB-CG	6.50	119.10	112.60
1	A	41	THR	CA-CB-OG1	-6.48	99.88	109.60
2	D	37	TRP	CG-CD2-CE3	6.48	140.38	133.90
2	D	92	HIS	CB-CG-CD2	-6.48	122.78	131.20
2	D	130	PHE	CA-CB-CG	-6.46	107.34	113.80
2	B	71	PHE	CA-CB-CG	-6.45	107.35	113.80
1	A	103	HIS	N-CA-C	-6.40	104.22	111.07
2	D	22	GLU	CB-CG-CD	6.38	123.44	112.60
2	B	57	ASN	CA-C-O	-6.37	113.07	119.24
1	A	50	HIS	CB-CG-CD2	-6.36	122.93	131.20
1	C	132	VAL	CB-CA-C	-6.34	103.58	112.14
2	B	145	TYR	CA-C-O	-6.34	111.45	120.51
1	C	87	HIS	CA-C-O	-6.26	114.45	120.90
2	B	92	HIS	CB-CG-ND1	6.26	132.09	122.70
2	B	110	ILE	CA-CB-CG1	-6.26	99.76	110.40
2	D	60	VAL	N-CA-C	-6.24	104.42	110.72
2	B	139	ASN	CA-CB-CG	-6.20	106.40	112.60
2	D	129	ALA	N-CA-C	-6.19	104.45	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	95	GLN	OE1-CD-NE2	-6.19	116.41	122.60
1	A	110	ALA	O-C-N	6.17	128.43	122.07
1	A	47	ASN	OD1-CG-ND2	-6.16	116.44	122.60
2	D	77	HIS	CB-CG-CD2	-6.16	123.19	131.20
2	B	57	ASN	CA-C-N	6.14	126.31	119.32
2	B	57	ASN	C-N-CA	6.14	126.31	119.32
1	A	84	SER	CB-CA-C	-6.13	101.18	110.92
1	C	70	VAL	N-CA-C	-6.11	103.25	111.44
2	D	79	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	74	ASP	CA-CB-CG	6.11	118.70	112.60
2	B	65	LYS	CA-CB-CG	6.08	126.27	114.10
1	A	138	SER	O-C-N	-6.07	115.54	122.09
1	A	131	ASN	CB-CG-ND2	6.06	125.49	116.40
1	A	137	THR	CB-CA-C	6.06	121.06	110.64
2	D	48	LEU	CA-C-O	6.04	126.63	119.56
1	C	24	HIS	CA-C-O	-5.98	114.08	120.42
2	B	146	HIS	N-CA-CB	-5.97	100.35	110.50
1	A	47	ASN	CB-CG-ND2	5.95	125.32	116.40
1	C	36	PHE	O-C-N	-5.94	115.92	121.32
2	D	82	LYS	CB-CG-CD	5.94	124.96	111.30
2	D	6	GLU	CB-CG-CD	5.93	122.69	112.60
2	D	2	HIS	CB-CG-CD2	-5.93	123.50	131.20
2	D	30	ARG	NE-CZ-NH2	5.92	124.53	119.20
2	D	110	ILE	O-C-N	-5.92	116.12	121.87
1	C	9	ASN	CA-CB-CG	5.91	118.51	112.60
2	D	137	VAL	CA-C-O	-5.90	114.59	120.85
2	B	44	SER	N-CA-C	5.88	119.55	112.38
2	B	76	LYS	CA-C-N	5.88	132.77	121.54
2	B	76	LYS	C-N-CA	5.88	132.77	121.54
1	C	118	ASN	CA-C-N	5.86	125.73	119.28
1	C	118	ASN	C-N-CA	5.86	125.73	119.28
1	A	47	ASN	N-CA-C	-5.85	100.46	109.76
1	A	45	HIS	CE1-NE2-CD2	5.84	114.84	109.00
2	B	131	GLN	CB-CG-CD	5.83	122.52	112.60
2	D	94	ASP	CA-CB-CG	5.82	118.42	112.60
1	C	118	ASN	OD1-CG-ND2	-5.79	116.81	122.60
1	C	72	HIS	CA-CB-CG	5.79	119.58	113.80
1	C	64	ASP	N-CA-C	-5.78	105.06	111.36
2	D	31	LEU	N-CA-C	-5.78	104.88	111.07
1	C	138	SER	N-CA-C	5.78	118.35	111.71
1	A	116	ASP	CB-CA-C	5.76	116.59	109.16
2	B	40	ARG	CA-CB-CG	-5.75	102.60	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	HIS	CA-CB-CG	-5.72	108.08	113.80
1	C	103	HIS	CB-CG-CD2	-5.71	123.78	131.20
2	B	66	LYS	O-C-N	-5.70	115.66	122.15
1	A	24	HIS	CB-CG-CD2	-5.69	123.80	131.20
1	C	112	HIS	ND1-CG-CD2	5.68	111.78	106.10
2	B	110	ILE	CA-CB-CG2	5.67	120.14	110.50
2	D	57	ASN	N-CA-C	5.67	117.11	109.24
1	C	141	ARG	NE-CZ-NH2	-5.64	114.12	119.20
1	A	122	HIS	CA-C-O	-5.62	114.91	120.82
2	D	103	PHE	N-CA-C	-5.61	105.24	111.36
1	C	83	LEU	CA-C-O	-5.61	113.17	119.79
2	D	132	LYS	CA-C-O	5.61	126.36	120.42
1	C	73	LEU	N-CA-C	5.58	119.19	112.38
2	D	86	ALA	O-C-N	-5.58	116.33	122.07
1	A	90	LYS	CA-CB-CG	5.57	125.25	114.10
1	A	43	PHE	CA-C-O	-5.57	112.53	120.16
2	D	22	GLU	N-CA-C	-5.57	98.93	110.80
2	D	146	HIS	CB-CG-CD2	-5.57	123.96	131.20
2	B	146	HIS	ND1-CE1-NE2	-5.57	102.83	108.40
1	A	113	HIS	CB-CG-CD2	-5.56	123.97	131.20
2	D	110	ILE	N-CA-C	-5.54	104.97	110.62
1	C	43	PHE	CA-C-N	5.54	125.06	119.19
1	C	43	PHE	C-N-CA	5.54	125.06	119.19
2	D	11	VAL	O-C-N	-5.54	116.14	121.90
2	B	146	HIS	ND1-CG-CD2	-5.53	100.57	106.10
2	B	63	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	A	53	ASP	N-CA-C	-5.52	105.42	111.82
1	C	135	VAL	N-CA-C	-5.50	105.36	110.53
1	A	67	THR	O-C-N	-5.49	116.30	122.12
2	D	37	TRP	CE2-CD2-CG	-5.48	100.62	107.20
2	D	132	LYS	CB-CG-CD	-5.45	98.77	111.30
2	D	117	ARG	CA-CB-CG	-5.44	103.22	114.10
1	C	74	ASP	CA-CB-CG	5.44	118.04	112.60
2	D	123	ASN	CA-C-N	5.43	125.51	119.32
2	D	123	ASN	C-N-CA	5.43	125.51	119.32
1	A	89	HIS	N-CA-C	5.41	116.86	111.07
1	C	113	HIS	CA-C-N	5.40	125.48	119.32
1	C	113	HIS	C-N-CA	5.40	125.48	119.32
1	A	118	ASN	CA-C-N	5.40	125.47	119.32
1	A	118	ASN	C-N-CA	5.40	125.47	119.32
1	A	134	THR	CB-CA-C	-5.40	102.41	110.88
1	A	138	SER	N-CA-C	5.39	116.97	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	6	GLU	CA-CB-CG	5.39	124.89	114.10
1	A	24	HIS	O-C-N	5.39	127.84	122.12
1	C	133	SER	CA-C-O	-5.39	114.71	120.42
1	A	8	ALA	N-CA-C	5.38	118.64	111.75
1	C	124	SER	CA-C-O	-5.37	114.73	120.42
2	D	78	LEU	N-CA-C	5.37	118.62	111.75
1	C	112	HIS	CA-CB-CG	-5.34	108.46	113.80
2	B	84	THR	N-CA-C	-5.34	105.46	111.28
2	B	108	ASN	CA-CB-CG	-5.34	107.26	112.60
2	D	92	HIS	CB-CG-ND1	5.33	130.69	122.70
1	C	133	SER	CA-CB-OG	-5.32	100.47	111.10
2	B	129	ALA	N-CA-C	-5.31	105.41	111.14
2	D	18	VAL	N-CA-CB	-5.30	105.01	110.95
1	C	16	LYS	CA-CB-CG	5.30	124.71	114.10
1	A	109	LEU	CA-C-N	5.30	127.33	120.44
1	A	109	LEU	C-N-CA	5.30	127.33	120.44
1	C	130	ALA	N-CA-C	-5.30	105.59	111.36
1	A	127	LYS	CB-CA-C	-5.29	101.86	110.85
2	D	2	HIS	CB-CG-ND1	5.28	130.62	122.70
2	D	104	ARG	CA-CB-CG	5.28	124.65	114.10
2	D	65	LYS	CA-CB-CG	5.27	124.64	114.10
2	D	145	TYR	CA-CB-CG	-5.27	104.41	113.90
2	D	15	TRP	CG-CD2-CE3	5.26	139.16	133.90
2	B	100	PRO	N-CA-C	5.26	120.68	113.84
1	C	116	ASP	N-CA-C	5.25	119.75	113.23
2	B	111	VAL	O-C-N	-5.25	116.78	121.87
2	B	57	ASN	OD1-CG-ND2	-5.25	117.35	122.60
1	C	138	SER	O-C-N	-5.25	116.08	122.22
2	D	82	LYS	CG-CD-CE	5.25	123.37	111.30
2	B	104	ARG	O-C-N	-5.22	116.45	122.09
2	D	146	HIS	CA-CB-CG	5.22	119.02	113.80
1	C	17	VAL	N-CA-C	-5.22	105.41	110.42
1	C	89	HIS	CA-CB-CG	5.22	119.02	113.80
2	D	120	HIS	CB-CG-CD2	-5.22	124.42	131.20
2	D	145	TYR	O-C-N	5.20	129.56	122.48
1	A	62	VAL	N-CA-C	-5.20	105.47	110.72
2	B	137	VAL	N-CA-C	5.18	116.53	110.62
1	C	43	PHE	O-C-N	-5.17	115.37	121.32
1	C	123	ALA	CA-C-O	-5.17	115.07	120.55
1	C	23	ALA	O-C-N	-5.15	116.77	122.07
2	B	146	HIS	CB-CG-ND1	5.14	130.42	122.70
1	C	67	THR	CA-CB-OG1	-5.13	101.91	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	47	ASN	N-CA-C	-5.12	100.90	109.24
2	D	18	VAL	CA-CB-CG2	-5.11	101.71	110.40
1	A	101	LEU	O-C-N	-5.11	116.71	122.12
1	A	14	TRP	CB-CG-CD1	-5.10	119.25	126.90
1	A	81	SER	O-C-N	-5.09	116.27	122.22
1	A	20	GLN	OE1-CD-NE2	-5.09	117.51	122.60
2	B	2	HIS	CB-CG-CD2	-5.05	124.63	131.20
1	A	27	GLU	N-CA-C	-5.04	105.70	111.14
1	A	75	ASP	CA-CB-CG	5.04	117.64	112.60
2	B	77	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	C	141	ARG	N-CA-CB	-5.03	101.95	110.50
1	C	118	ASN	CA-CB-CG	5.02	117.62	112.60
2	D	111	VAL	O-C-N	-5.01	116.13	121.80
1	A	112	HIS	O-C-N	-5.01	115.60	122.46
2	B	76	LYS	CA-CB-CG	5.00	124.11	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	145	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	1064	0	1060	27	0
1	C	1064	0	1060	22	0
2	B	1135	0	1134	28	0
2	D	1135	0	1134	25	0
3	A	43	0	30	0	0
3	B	43	0	30	1	0
3	C	43	0	30	2	0
3	D	43	0	30	4	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	A	104	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	143	0	0	0	0
5	C	135	0	0	2	0
5	D	192	0	0	3	0
All	All	5148	0	4508	91	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 10.

All (91) 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)
2:B:22:GLU:HB2	2:B:117:ARG:HH21	1.42	0.83
2:D:89:SER:HB2	2:D:144:LYS:HB2	1.58	0.82
1:A:6:ASP:O	1:A:10:VAL:HG23	1.83	0.79
2:B:146:HIS:HB3	2:D:132:LYS:HG2	1.68	0.74
1:C:72:HIS:HB3	1:C:75:ASP:HB3	1.72	0.71
1:C:76:LEU:HB3	1:C:77:PRO:HD3	1.73	0.70
1:C:98:PHE:HD1	3:C:850:HEM:HBB2	1.62	0.63
2:B:22:GLU:HB2	2:B:117:ARG:NH2	2.11	0.63
2:D:91:LEU:HD23	2:D:92:HIS:CE1	2.39	0.58
2:D:98:VAL:HG13	3:D:950:HEM:HBC2	1.84	0.58
1:A:107:VAL:HG13	2:B:115:ALA:HB2	1.86	0.56
1:C:1:VAL:HG12	1:C:2:LEU:H	1.70	0.56
2:B:5:ALA:O	2:B:9:GLU:HG3	2.06	0.56
1:A:133:SER:O	1:A:137:THR:HB	2.05	0.56
2:B:62:ALA:O	2:B:65:LYS:HG3	2.06	0.55
1:A:34:LEU:HD12	2:B:124:PRO:CB	2.36	0.55
1:A:122:HIS:HD2	2:B:30:ARG:HD3	1.71	0.55
1:C:21:ALA:HB1	1:C:63:ALA:HB1	1.89	0.55
1:C:103:HIS:HD2	5:C:862:HOH:O	1.88	0.55
2:D:89:SER:HB3	2:D:141:LEU:O	2.07	0.54
1:A:140:TYR:HB2	5:A:692:HOH:O	2.08	0.54
2:B:106:LEU:HD23	3:B:750:HEM:HAB	1.90	0.54
2:B:59:LYS:HD2	2:B:59:LYS:N	2.24	0.53
1:A:96:VAL:O	1:A:99:LYS:HG2	2.09	0.53
2:D:14:LEU:HD23	2:D:126:VAL:HG11	1.91	0.52
2:B:145:TYR:O	2:B:146:HIS:HD2	1.93	0.51
1:A:7:LYS:O	1:A:11:LYS:HG2	2.11	0.51
2:D:91:LEU:O	2:D:96:LEU:HG	2.11	0.50
1:A:127:LYS:HD3	1:C:141:ARG:HA	1.93	0.50
2:B:104:ARG:N	2:B:104:ARG:HD3	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:HIS:HB3	1:A:93:VAL:HG13	1.92	0.50
1:A:139:LYS:N	1:A:139:LYS:HD2	2.26	0.50
1:A:140:TYR:HB3	2:D:36:PRO:HG2	1.92	0.50
2:B:57:ASN:O	2:B:61:LYS:HG2	2.11	0.50
1:C:1:VAL:HG11	1:C:73:LEU:O	2.12	0.49
1:A:16:LYS:HG2	1:A:116:ASP:OD2	2.13	0.49
1:A:95:PRO:HD3	1:A:140:TYR:OH	2.12	0.49
1:A:68:LYS:O	1:A:72:HIS:HD2	1.97	0.48
2:D:123:ASN:OD1	2:D:126:VAL:HG23	2.14	0.48
1:C:132:VAL:O	1:C:136:LEU:HD12	2.15	0.47
2:D:141:LEU:CD1	3:D:950:HEM:HAB	2.44	0.47
1:C:68:LYS:HD2	5:C:910:HOH:O	2.15	0.47
1:A:32:MET:HE3	1:A:39:THR:HB	1.96	0.46
1:C:68:LYS:O	1:C:72:HIS:HD2	1.99	0.46
2:B:122:PHE:HA	2:B:126:VAL:HG21	1.98	0.46
1:C:98:PHE:CD1	3:C:850:HEM:HBB2	2.48	0.46
1:A:34:LEU:HD12	2:B:124:PRO:HB2	1.97	0.46
1:C:88:ALA:CB	1:C:139:LYS:HB2	2.45	0.46
2:D:20:VAL:HG22	2:D:68:LEU:HD23	1.98	0.46
2:D:91:LEU:HD22	3:D:950:HEM:HBA2	1.97	0.45
2:D:12:LEU:HD23	5:D:1137:HOH:O	2.15	0.45
2:D:26:GLU:O	2:D:30:ARG:HG3	2.15	0.45
2:B:71:PHE:CE1	2:B:137:VAL:HG21	2.52	0.45
2:B:3:LEU:HD12	2:B:8:LYS:HG2	1.99	0.45
2:B:146:HIS:CE1	1:C:37:PRO:HG2	2.52	0.45
1:C:105:LEU:O	1:C:109:LEU:HG	2.16	0.45
1:A:113:HIS:HB3	1:A:116:ASP:HB3	1.98	0.45
2:D:43:GLU:HG2	5:D:1051:HOH:O	2.17	0.44
2:D:2:HIS:HB2	5:D:1036:HOH:O	2.16	0.44
2:B:142:ALA:O	2:B:145:TYR:HB2	2.18	0.44
2:B:30:ARG:O	2:B:34:VAL:HG23	2.17	0.44
1:A:63:ALA:HA	1:A:66:LEU:HD12	2.00	0.43
2:B:145:TYR:O	2:B:146:HIS:CD2	2.71	0.43
2:D:57:ASN:HA	2:D:58:PRO:HD3	1.85	0.43
2:B:29:GLY:O	2:B:33:VAL:HG12	2.18	0.43
1:C:33:PHE:CE2	1:C:48:LEU:HD22	2.53	0.43
1:A:66:LEU:O	1:A:70:VAL:HG23	2.18	0.43
1:A:76:LEU:N	1:A:77:PRO:CD	2.82	0.42
1:C:2:LEU:HD21	1:C:131:ASN:ND2	2.33	0.42
1:C:72:HIS:CD2	1:C:72:HIS:N	2.88	0.42
2:D:14:LEU:CD2	2:D:126:VAL:HG11	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:HIS:HE1	2:D:131:GLN:OE1	2.02	0.42
1:C:94:ASP:HA	1:C:95:PRO:HD3	1.89	0.42
2:D:91:LEU:CD2	3:D:950:HEM:HBA2	2.50	0.42
2:B:92:HIS:CD2	2:B:96:LEU:HD12	2.55	0.41
1:A:103:HIS:HE1	2:B:131:GLN:OE1	2.03	0.41
5:A:654:HOH:O	2:D:41:PHE:HZ	2.03	0.41
1:C:41:THR:O	1:C:44:PRO:HD3	2.20	0.41
2:D:107:GLY:HA3	2:D:134:VAL:HG13	2.03	0.41
2:B:14:LEU:HD22	2:B:130:PHE:CE2	2.55	0.41
1:A:34:LEU:HD12	2:B:124:PRO:HB3	2.03	0.41
1:A:60:GLN:HG2	5:A:749:HOH:O	2.21	0.40
2:D:65:LYS:HB2	2:D:65:LYS:HE3	1.59	0.40
1:A:33:PHE:CE2	1:A:48:LEU:HD22	2.57	0.40
1:C:2:LEU:HB3	1:C:6:ASP:HB2	2.01	0.40
2:D:42:PHE:O	2:D:45:PHE:HB2	2.21	0.40
1:A:139:LYS:HA	5:A:718:HOH:O	2.21	0.40
1:A:2:LEU:HD23	1:A:2:LEU:HA	1.97	0.40
2:B:56:GLY:H	2:B:61:LYS:HD3	1.86	0.40
2:B:68:LEU:HA	2:B:68:LEU:HD22	1.84	0.40
2:D:19:ASN:CG	2:D:22:GLU:HB2	2.46	0.40

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	139/141 (99%)	130 (94%)	7 (5%)	2 (1%)	9 2
1	C	139/141 (99%)	135 (97%)	3 (2%)	1 (1%)	18 8
2	B	144/146 (99%)	136 (94%)	6 (4%)	2 (1%)	9 2
2	D	144/146 (99%)	132 (92%)	12 (8%)	0	100 100
All	All	566/574 (99%)	533 (94%)	28 (5%)	5 (1%)	14 5

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	77	HIS
2	B	145	TYR
1	A	43	PHE
1	A	37	PRO
1	C	43	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	111/111 (100%)	97 (87%)	14 (13%)	4	1
1	C	111/111 (100%)	99 (89%)	12 (11%)	6	1
2	B	119/119 (100%)	94 (79%)	25 (21%)	1	0
2	D	119/119 (100%)	103 (87%)	16 (13%)	4	1
All	All	460/460 (100%)	393 (85%)	67 (15%)	3	1

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	53	ASP
1	A	56	LYS
1	A	76	LEU
1	A	86	LEU
1	A	89	HIS
1	A	90	LYS
1	A	92	ARG
1	A	93	VAL
1	A	99	LYS
1	A	105	LEU
1	A	120	SER
1	A	129	LEU
1	A	137	THR
2	B	3	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	12	LEU
2	B	18	VAL
2	B	23	VAL
2	B	33	VAL
2	B	43	GLU
2	B	49	SER
2	B	65	LYS
2	B	66	LYS
2	B	67	VAL
2	B	68	LEU
2	B	69	GLN
2	B	75	LEU
2	B	76	LYS
2	B	78	LEU
2	B	91	LEU
2	B	101	GLU
2	B	104	ARG
2	B	110	ILE
2	B	112	VAL
2	B	117	ARG
2	B	132	LYS
2	B	134	VAL
2	B	139	ASN
2	B	144	LYS
1	C	2	LEU
1	C	16	LYS
1	C	20	GLN
1	C	34	LEU
1	C	52	SER
1	C	72	HIS
1	C	92	ARG
1	C	96	VAL
1	C	106	LEU
1	C	115	ASP
1	C	131	ASN
1	C	139	LYS
2	D	6	GLU
2	D	22	GLU
2	D	40	ARG
2	D	59	LYS
2	D	66	LYS
2	D	68	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	71	PHE
2	D	76	LYS
2	D	78	LEU
2	D	82	LYS
2	D	87	LYS
2	D	88	LEU
2	D	89	SER
2	D	134	VAL
2	D	144	LYS
2	D	146	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	89	HIS
1	A	103	HIS
1	A	112	HIS
1	A	122	HIS
2	B	146	HIS
1	C	72	HIS
1	C	103	HIS
1	C	112	HIS
1	C	131	ASN
2	D	80	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

6 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	HEM	B	750	4	50,50,50	1.28	5 (10%)	67,82,82	1.22	7 (10%)
4	OXY	C	851	3	1,1,1	0.13	0	-		
4	OXY	B	751	3	1,1,1	0.12	0	-		
3	HEM	A	650	5,1	50,50,50	1.38	10 (20%)	67,82,82	1.28	7 (10%)
3	HEM	D	950	5	50,50,50	1.39	9 (18%)	67,82,82	1.40	8 (11%)
3	HEM	C	850	4	50,50,50	1.35	5 (10%)	67,82,82	1.31	10 (14%)

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	HEM	D	950	5	-	8/14/54/54	-
3	HEM	B	750	4	-	5/14/54/54	-
3	HEM	C	850	4	-	7/14/54/54	-
3	HEM	A	650	5,1	-	8/14/54/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	850	HEM	CBB-CAB	4.22	1.50	1.30
3	C	850	HEM	CBC-CAC	4.12	1.50	1.30
3	A	650	HEM	CBC-CAC	3.83	1.48	1.30
3	D	950	HEM	CBC-CAC	3.82	1.48	1.30
3	D	950	HEM	CBB-CAB	3.50	1.47	1.30
3	A	650	HEM	CBB-CAB	3.16	1.45	1.30
3	B	750	HEM	CBB-CAB	2.90	1.44	1.30
3	A	650	HEM	CAC-C3C	-2.62	1.40	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	850	HEM	CAC-C3C	-2.55	1.40	1.47
3	B	750	HEM	CBC-CAC	2.53	1.42	1.30
3	A	650	HEM	C1D-ND	2.52	1.43	1.38
3	B	750	HEM	C3C-C4C	2.51	1.50	1.46
3	D	950	HEM	C1D-C2D	2.42	1.49	1.44
3	A	650	HEM	CAB-C3B	-2.34	1.41	1.47
3	C	850	HEM	C2A-C3A	-2.29	1.32	1.38
3	D	950	HEM	CAB-C3B	-2.26	1.41	1.47
3	A	650	HEM	C3B-C4B	2.26	1.49	1.44
3	B	750	HEM	CAB-C3B	-2.25	1.41	1.47
3	A	650	HEM	O2D-CGD	-2.22	1.23	1.30
3	A	650	HEM	CMD-C2D	2.21	1.55	1.50
3	D	950	HEM	C4D-C3D	2.21	1.48	1.45
3	D	950	HEM	CAC-C3C	-2.19	1.41	1.47
3	D	950	HEM	C3C-C2C	-2.09	1.32	1.37
3	B	750	HEM	C1C-C2C	2.09	1.49	1.45
3	C	850	HEM	C3C-C4C	2.08	1.49	1.46
3	A	650	HEM	CHA-C4D	2.06	1.42	1.38
3	D	950	HEM	O2D-CGD	-2.03	1.24	1.30
3	A	650	HEM	O2A-CGA	-2.02	1.24	1.30
3	D	950	HEM	C4A-C3A	2.02	1.47	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	950	HEM	C3B-C4B-NB	3.40	111.91	109.47
3	B	750	HEM	C4D-ND-C1D	-3.29	101.31	105.21
3	B	750	HEM	C3B-C4B-NB	3.27	111.82	109.47
3	A	650	HEM	C2D-C1D-ND	3.05	113.43	109.90
3	D	950	HEM	C3D-C4D-ND	2.95	113.40	110.17
3	D	950	HEM	C4D-ND-C1D	-2.89	101.79	105.21
3	D	950	HEM	C4A-NA-C1A	-2.77	101.30	105.82
3	C	850	HEM	O1D-CGD-CBD	-2.74	114.39	123.09
3	A	650	HEM	CHC-C1C-NC	-2.74	121.47	124.45
3	D	950	HEM	C2A-C1A-NA	2.73	113.18	110.15
3	C	850	HEM	CAA-CBA-CGA	-2.73	106.42	113.67
3	A	650	HEM	C4B-C3B-C2B	-2.66	104.83	107.28
3	A	650	HEM	C3B-C4B-NB	2.64	111.36	109.47
3	B	750	HEM	C4B-C3B-C2B	-2.47	105.01	107.28
3	C	850	HEM	CHD-C4C-NC	-2.43	121.81	124.45
3	D	950	HEM	C4C-NC-C1C	-2.40	101.91	105.82
3	A	650	HEM	C1D-C2D-C3D	-2.35	104.51	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	750	HEM	O1D-CGD-CBD	-2.34	115.67	123.09
3	C	850	HEM	C2B-C1B-NB	2.29	112.47	109.84
3	A	650	HEM	C4D-ND-C1D	-2.28	102.50	105.21
3	A	650	HEM	C2B-C1B-NB	2.26	112.44	109.84
3	C	850	HEM	CMD-C2D-C1D	2.25	128.55	125.03
3	C	850	HEM	C2D-C1D-ND	2.23	112.48	109.90
3	C	850	HEM	C1D-C2D-C3D	-2.22	104.64	106.98
3	D	950	HEM	CMC-C2C-C1C	2.21	128.62	124.73
3	C	850	HEM	O2D-CGD-CBD	2.16	120.84	114.00
3	B	750	HEM	CHD-C4C-C3C	-2.16	121.57	125.21
3	B	750	HEM	C4C-C3C-C2C	-2.11	104.99	106.81
3	B	750	HEM	CAD-CBD-CGD	-2.08	108.14	113.67
3	D	950	HEM	CMB-C2B-C1B	2.07	128.26	125.03
3	C	850	HEM	CHC-C1C-NC	-2.04	122.23	124.45
3	C	850	HEM	CAD-C3D-C2D	-2.02	124.08	127.87

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	650	HEM	C2B-C3B-CAB-CBB
3	C	850	HEM	C2C-C3C-CAC-CBC
3	D	950	HEM	C2B-C3B-CAB-CBB
3	D	950	HEM	C4B-C3B-CAB-CBB
3	D	950	HEM	C2C-C3C-CAC-CBC
3	A	650	HEM	C4B-C3B-CAB-CBB
3	C	850	HEM	C4C-C3C-CAC-CBC
3	D	950	HEM	C4C-C3C-CAC-CBC
3	A	650	HEM	C2A-CAA-CBA-CGA
3	D	950	HEM	CAD-CBD-CGD-O1D
3	A	650	HEM	CAD-CBD-CGD-O1D
3	C	850	HEM	CAA-CBA-CGA-O2A
3	B	750	HEM	CAD-CBD-CGD-O1D
3	D	950	HEM	CAD-CBD-CGD-O2D
3	A	650	HEM	CAD-CBD-CGD-O2D
3	C	850	HEM	CAA-CBA-CGA-O1A
3	B	750	HEM	CAD-CBD-CGD-O2D
3	A	650	HEM	CAA-CBA-CGA-O2A
3	B	750	HEM	CAA-CBA-CGA-O1A
3	B	750	HEM	CAA-CBA-CGA-O2A
3	A	650	HEM	CAA-CBA-CGA-O1A
3	C	850	HEM	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

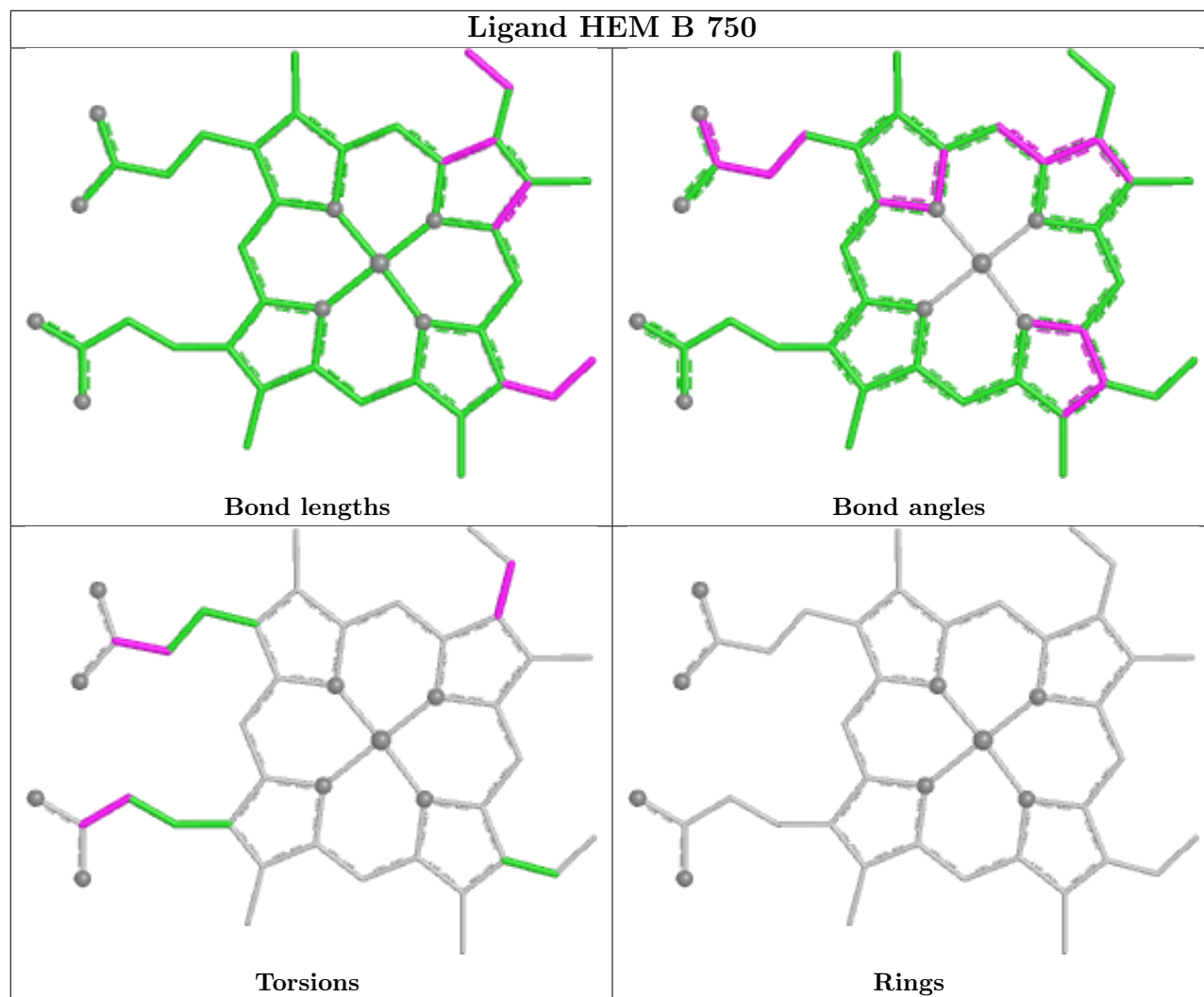
Mol	Chain	Res	Type	Atoms
3	C	850	HEM	CAD-CBD-CGD-O2D
3	D	950	HEM	CAA-CBA-CGA-O2A
3	A	650	HEM	C2C-C3C-CAC-CBC
3	B	750	HEM	C2C-C3C-CAC-CBC
3	C	850	HEM	CAD-CBD-CGD-O1D
3	D	950	HEM	CAA-CBA-CGA-O1A

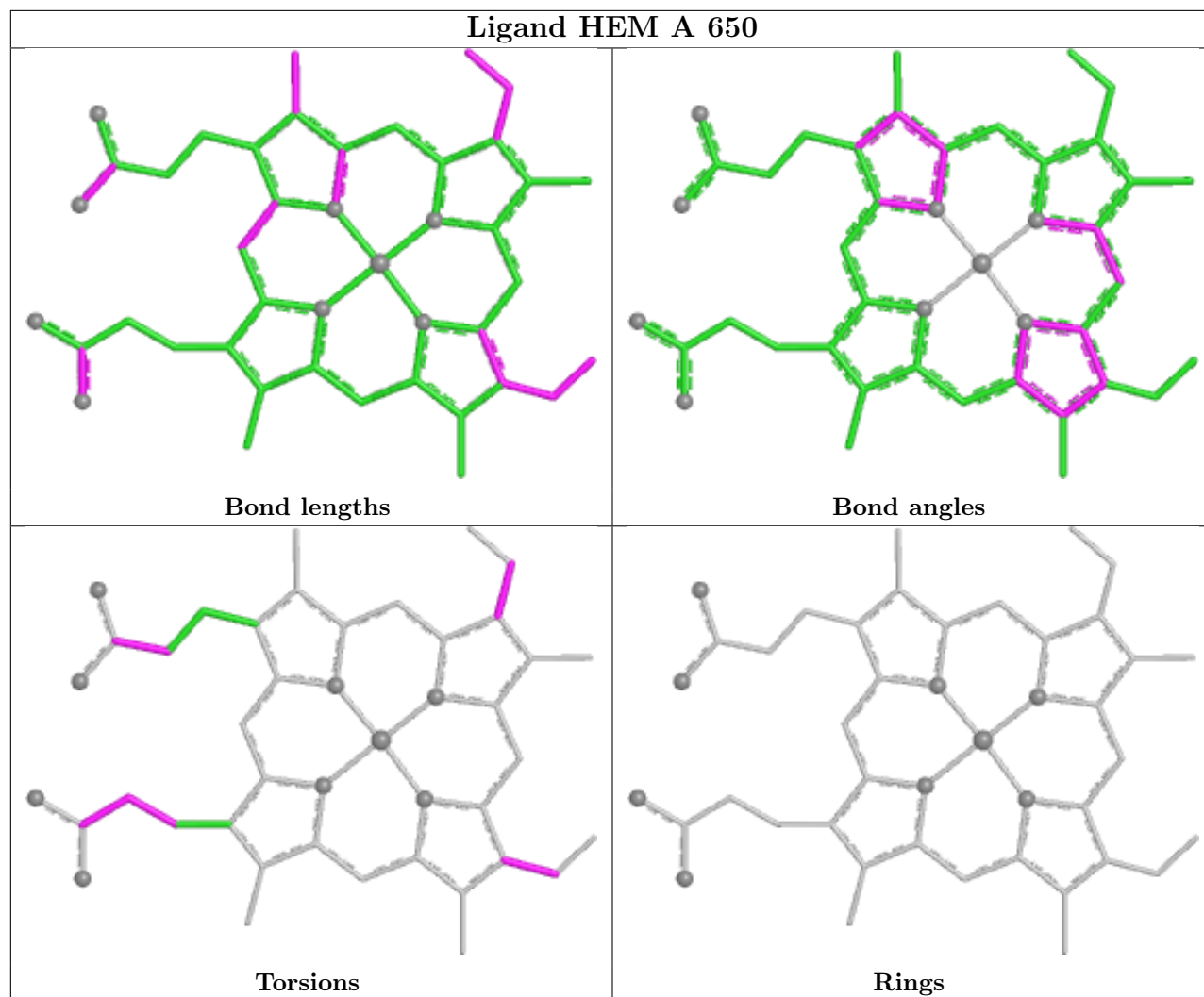
There are no ring outliers.

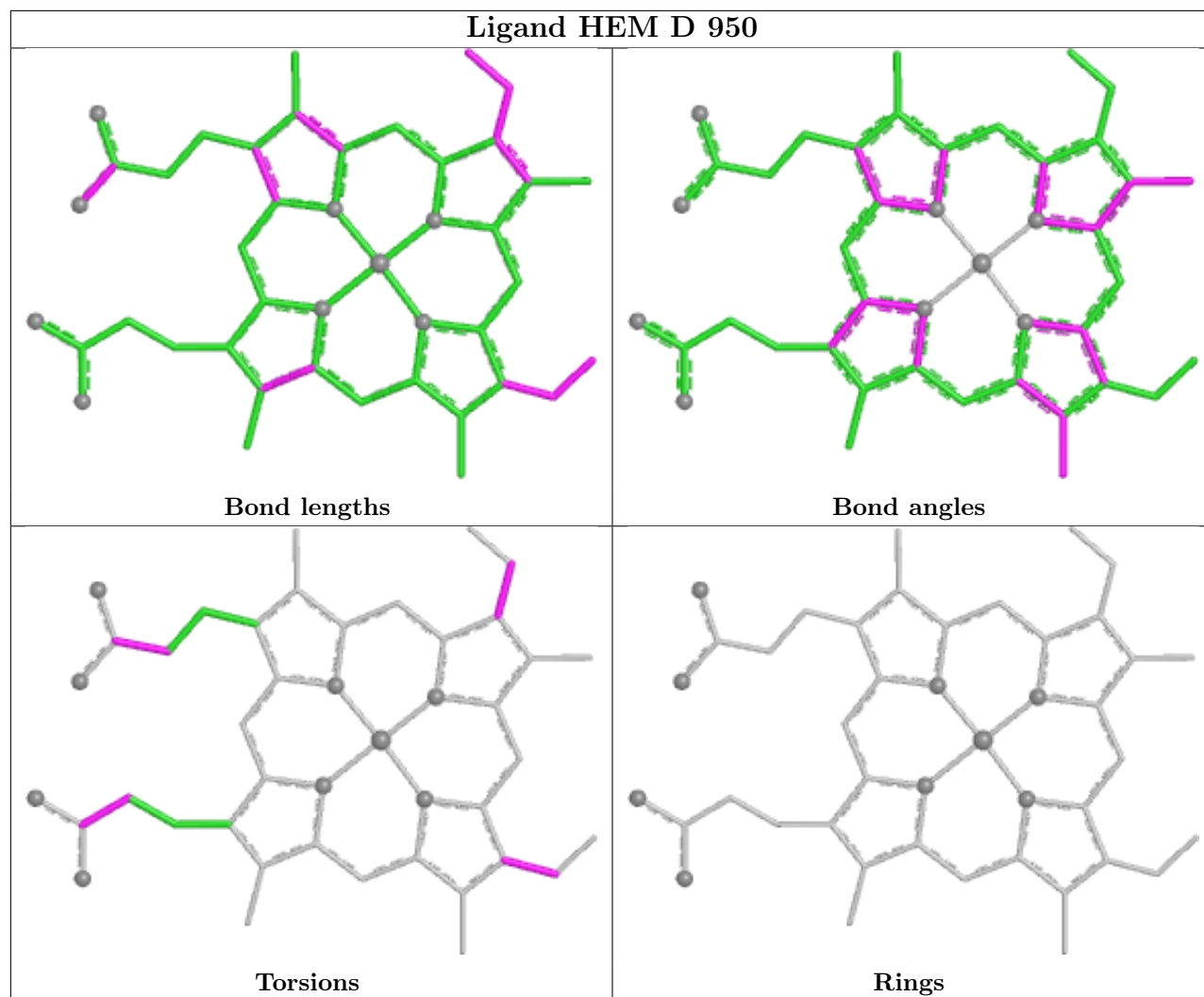
3 monomers are involved in 7 short contacts:

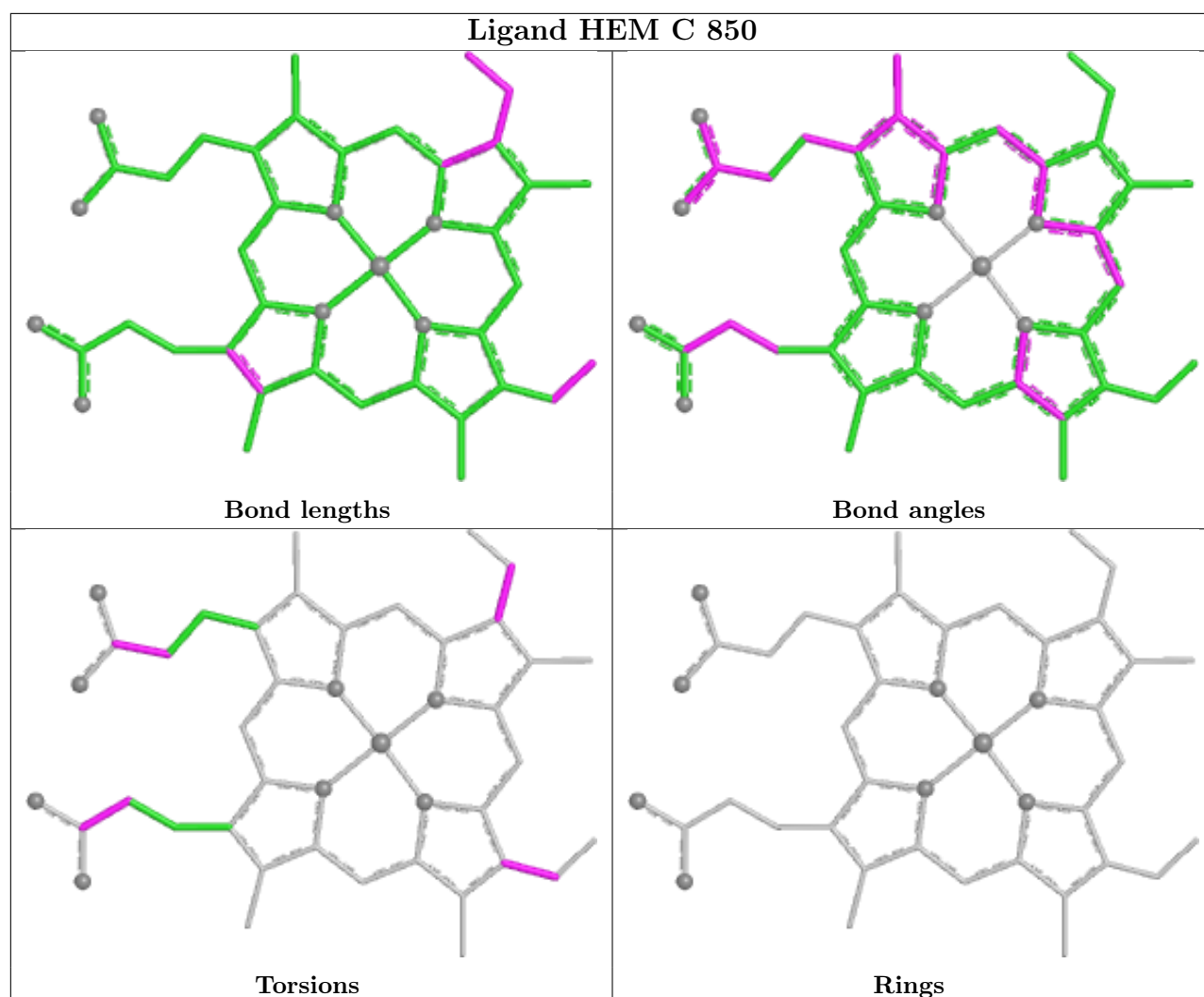
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	750	HEM	1	0
3	D	950	HEM	4	0
3	C	850	HEM	2	0

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	141/141 (100%)	-0.65	0 100 100	17, 30, 49, 61	0
1	C	141/141 (100%)	-0.67	0 100 100	16, 27, 44, 62	0
2	B	146/146 (100%)	-0.52	0 100 100	18, 35, 53, 61	0
2	D	146/146 (100%)	-0.69	0 100 100	11, 32, 49, 66	0
All	All	574/574 (100%)	-0.63	0 100 100	11, 32, 50, 66	0

There are no RSRZ outliers to report.

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
4	OXY	B	751	2/2	0.77	0.29	40,40,40,41	0
3	HEM	D	950	43/43	0.90	0.08	36,45,60,65	0
4	OXY	C	851	2/2	0.92	0.25	36,36,36,37	0
3	HEM	B	750	43/43	0.94	0.06	29,36,54,65	0

Continued on next page...

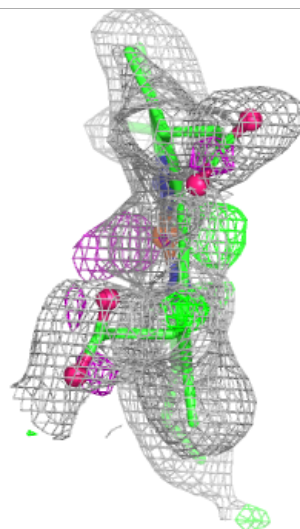
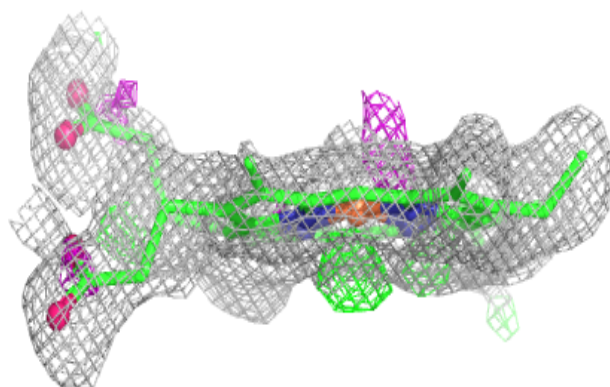
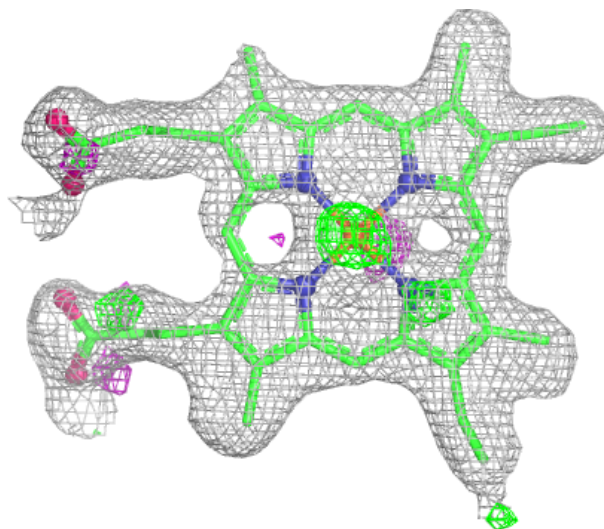
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEM	C	850	43/43	0.96	0.05	11,26,44,52	0
3	HEM	A	650	43/43	0.97	0.05	19,28,39,42	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.

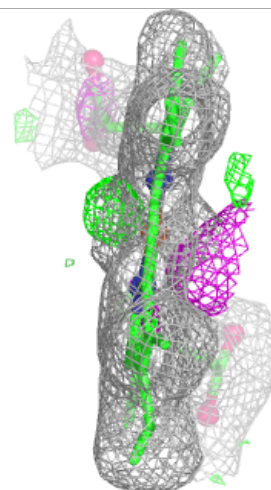
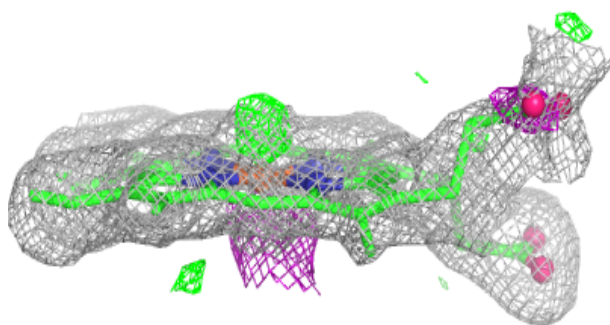
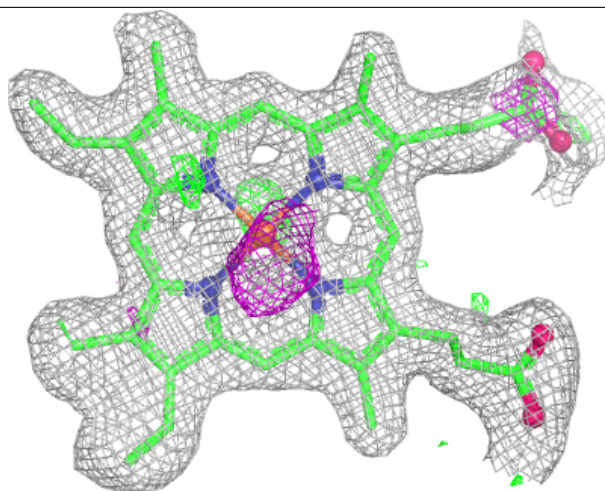
Electron density around HEM D 950:

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



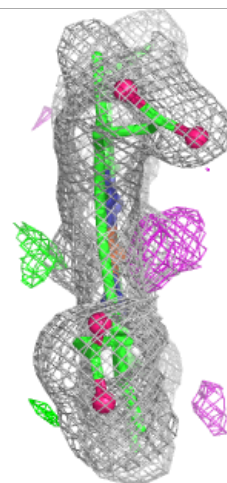
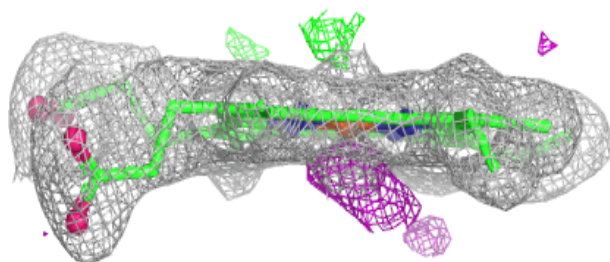
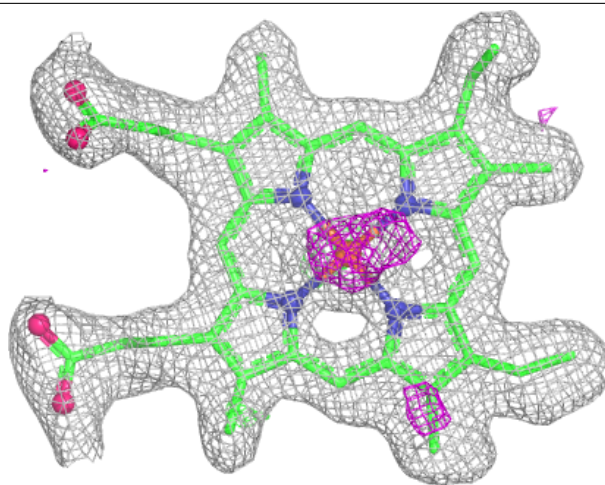
Electron density around HEM B 750:

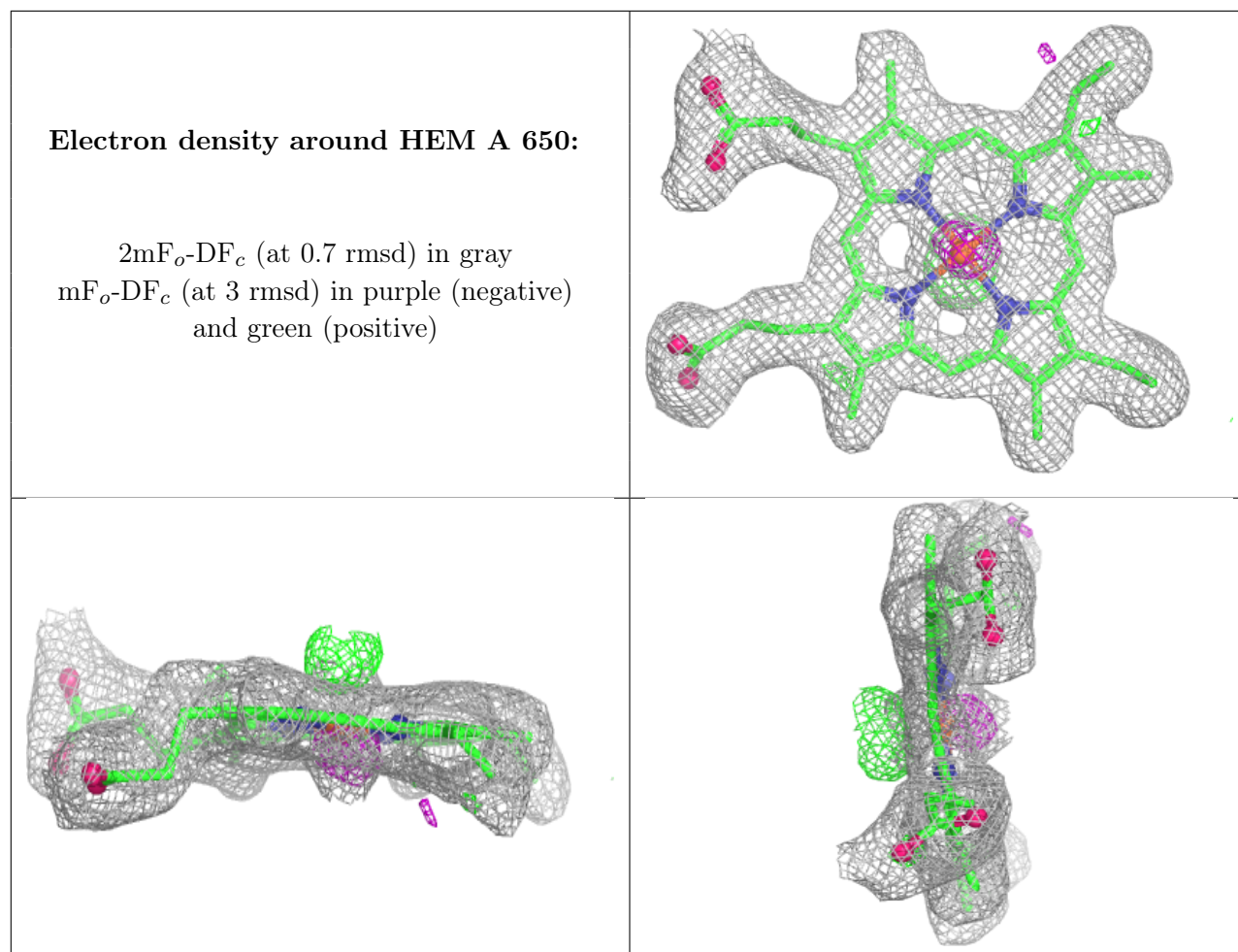
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 850:

$2mF_o-DF_c$ (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.