



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 05:51 AM EDT

PDB ID : 1OUU / pdb_00001ouu
Title : CARBONMONOXY TROUT HEMOGLOBIN I
Authors : Tame, J.; Wilson, J.
Deposited on : 1996-06-21
Resolution : 2.50 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

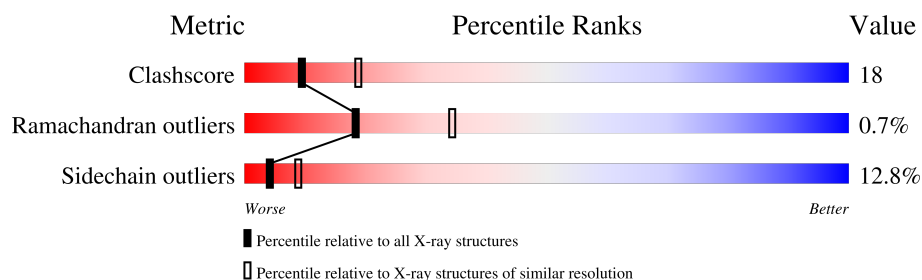
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	143	
1	C	143	
2	B	146	
2	D	146	

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
4	CMO	A	144	-	-	X	-
4	CMO	C	144	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4717 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 HEMOGLOBIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	0	0	0
			1066	690	181	191	4			
1	C	143	Total	C	N	O	S	0	0	0
			1066	690	181	191	4			

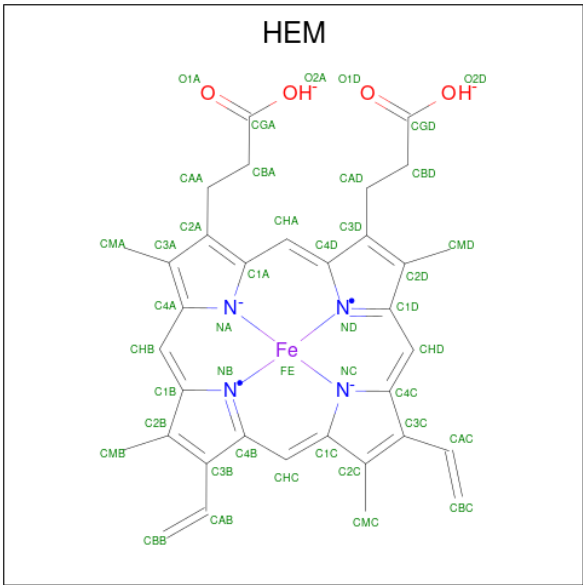
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP P02019
A	?	-	LYS	deletion	UNP P02019
C	?	-	ASP	deletion	UNP P02019
C	?	-	LYS	deletion	UNP P02019

- Molecule 2 is a protein called HEMOGLOBIN I.

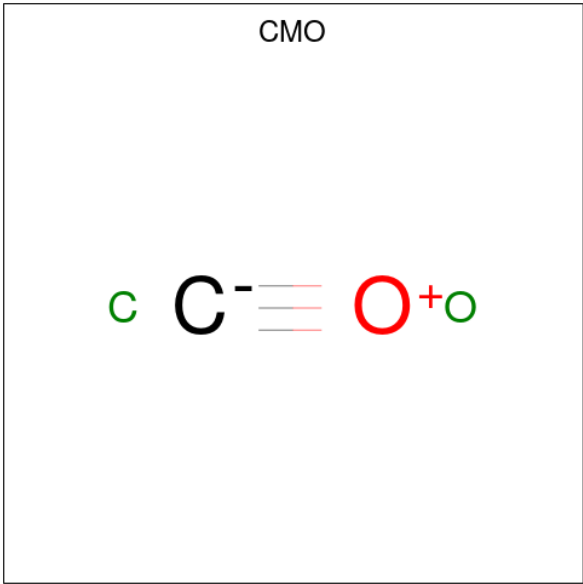
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1121	729	187	200	5			
2	D	146	Total	C	N	O	S	0	0	0
			1121	729	187	200	5			

- 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	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



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

- Molecule 5 is water.

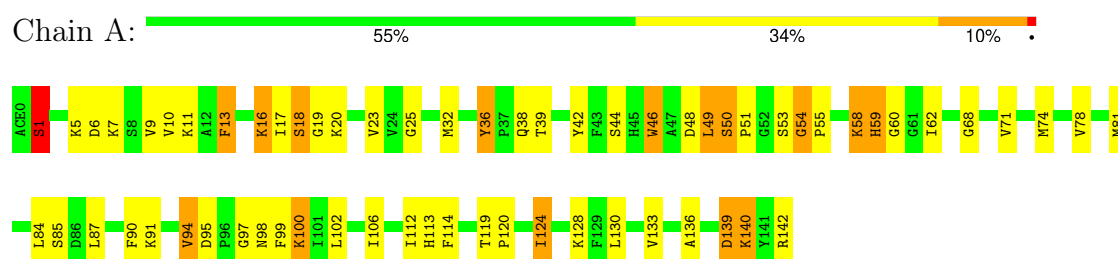
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	52	Total O 52 52	0	0
5	B	29	Total O 29 29	0	0
5	C	50	Total O 50 50	0	0
5	D	32	Total O 32 32	0	0

3 Residue-property plots

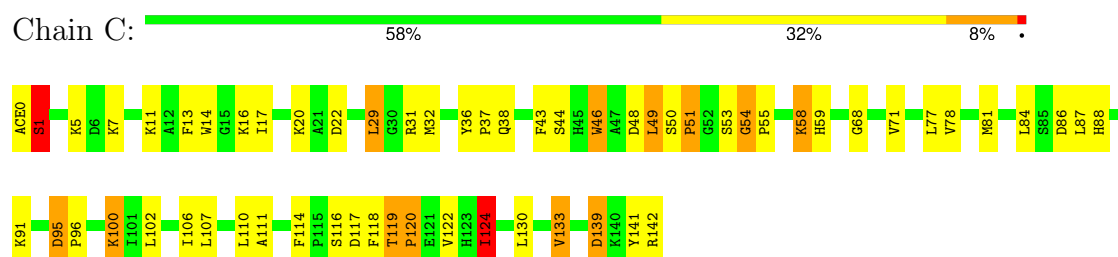
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

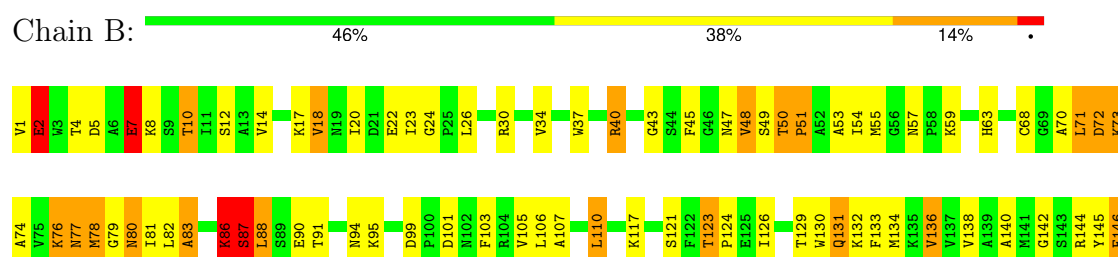
• Molecule 1: HEMOGLOBIN I



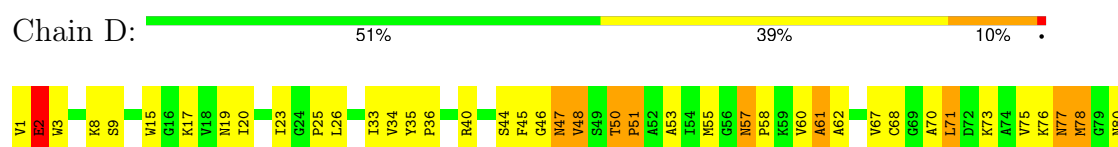
• Molecule 1: HEMOGLOBIN I



• Molecule 2: HEMOGLOBIN I



• Molecule 2: HEMOGLOBIN I



I81	L82	A83	T84	Y85	K86	S87	L88		T91	H92	A93	N94	K95	L96	F97	V98	D99		R104	V105	L106	A107		L110		A116	K117		T123	P124		A128	T129		K132	F133	M134	K135		A140		S143	R144	Y145	F146
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.20Å 79.80Å 122.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.162 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4717	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

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: ACE, CMO, 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	0.92	0/1089	1.90	30/1472 (2.0%)
1	C	0.91	0/1089	1.92	30/1472 (2.0%)
2	B	0.97	0/1148	2.06	48/1560 (3.1%)
2	D	0.95	1/1148 (0.1%)	2.14	49/1560 (3.1%)
All	All	0.94	1/4474 (0.0%)	2.01	157/6064 (2.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	77	ASN	CA-CB	5.59	1.60	1.53

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	47	ASN	CA-C-N	14.12	142.11	121.77
2	D	47	ASN	C-N-CA	14.12	142.11	121.77
2	D	47	ASN	CA-C-O	12.88	136.00	121.58
2	D	57	ASN	CA-C-O	11.04	129.59	119.76
2	D	19	ASN	CA-CB-CG	9.81	122.41	112.60
2	B	30	ARG	CD-NE-CZ	9.22	137.30	124.40
2	D	44	SER	N-CA-C	8.95	123.46	112.54
2	D	124	PRO	CA-C-N	8.81	131.90	120.44
2	D	124	PRO	C-N-CA	8.81	131.90	120.44
2	D	46	GLY	N-CA-C	8.11	123.32	111.24
1	A	139	ASP	N-CA-C	8.06	120.06	111.28
1	C	36	TYR	CA-C-N	7.90	128.09	119.87
1	C	36	TYR	C-N-CA	7.90	128.09	119.87
2	D	48	VAL	N-CA-CB	-7.71	100.35	112.07
2	B	144	ARG	CA-C-O	7.70	129.03	119.95
2	B	45	PHE	N-CA-C	7.64	122.42	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	94	ASN	N-CA-C	7.57	122.62	113.23
2	B	126	ILE	N-CA-C	-7.54	103.58	111.58
2	B	88	LEU	N-CA-C	-7.54	103.14	111.36
2	B	72	ASP	CA-CB-CG	-7.45	105.15	112.60
2	D	77	ASN	CA-CB-CG	-7.32	105.28	112.60
1	A	23	VAL	CB-CA-C	-7.27	102.19	112.22
2	B	43	GLY	N-CA-C	7.15	121.92	112.77
1	A	114	PHE	CA-C-N	7.10	127.09	119.28
1	A	114	PHE	C-N-CA	7.10	127.09	119.28
1	C	117	ASP	CA-CB-CG	-7.09	105.51	112.60
2	B	50	THR	CA-C-N	7.06	126.55	118.85
2	B	50	THR	C-N-CA	7.06	126.55	118.85
2	B	48	VAL	CA-C-N	7.03	130.65	120.38
2	B	48	VAL	C-N-CA	7.03	130.65	120.38
2	B	86	LYS	N-CA-C	6.96	118.95	111.36
1	C	114	PHE	CA-C-N	6.70	126.96	119.32
1	C	114	PHE	C-N-CA	6.70	126.96	119.32
1	C	29	LEU	CA-C-N	6.70	127.53	120.03
1	C	29	LEU	C-N-CA	6.70	127.53	120.03
2	B	94	ASN	CA-CB-CG	-6.67	105.93	112.60
1	C	124	ILE	CB-CA-C	-6.65	103.46	111.97
2	D	80	ASN	CA-CB-CG	-6.63	105.97	112.60
1	C	86	ASP	CB-CA-C	-6.58	99.67	110.85
2	B	83	ALA	CA-C-N	6.51	129.30	120.38
2	B	83	ALA	C-N-CA	6.51	129.30	120.38
2	B	130	TRP	CA-C-O	6.50	127.44	120.55
1	A	19	GLY	N-CA-C	6.37	120.60	112.83
2	B	71	LEU	CA-C-O	6.37	127.30	120.10
1	A	39	THR	CA-C-O	6.36	127.20	119.31
2	D	85	TYR	N-CA-C	6.32	119.71	112.57
2	B	110	LEU	CA-C-N	6.29	128.62	120.44
2	B	110	LEU	C-N-CA	6.29	128.62	120.44
1	A	38	GLN	CB-CG-CD	6.26	123.24	112.60
2	D	57	ASN	CA-C-N	6.24	127.64	119.84
2	D	57	ASN	C-N-CA	6.24	127.64	119.84
1	C	31	ARG	CD-NE-CZ	6.21	133.09	124.40
2	D	48	VAL	CA-C-O	6.15	125.72	119.20
2	B	2	GLU	CA-C-N	-6.15	114.51	123.00
2	B	2	GLU	C-N-CA	-6.15	114.51	123.00
1	A	139	ASP	CA-CB-CG	-6.13	106.47	112.60
2	B	123	THR	CA-C-N	6.03	126.19	119.32
2	B	123	THR	C-N-CA	6.03	126.19	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	15	TRP	CA-C-N	6.02	127.67	120.14
2	D	15	TRP	C-N-CA	6.02	127.67	120.14
1	C	22	ASP	CA-C-N	6.02	128.15	120.56
1	C	22	ASP	C-N-CA	6.02	128.15	120.56
2	D	2	GLU	CB-CG-CD	6.02	122.84	112.60
2	D	23	ILE	CA-C-O	-6.02	114.47	120.85
1	A	36	TYR	CA-C-N	6.01	125.69	119.56
1	A	36	TYR	C-N-CA	6.01	125.69	119.56
1	C	38	GLN	CB-CG-CD	5.98	122.77	112.60
2	D	88	LEU	N-CA-C	-5.93	104.89	111.36
2	D	99	ASP	CA-CB-CG	-5.89	106.71	112.60
1	A	94	VAL	O-C-N	5.85	129.62	122.95
1	C	51	PRO	N-CA-CB	5.83	108.43	103.19
2	D	60	VAL	N-CA-C	-5.81	105.07	110.53
2	D	128	ALA	CA-C-O	-5.81	114.39	120.55
1	A	46	TRP	CA-C-N	5.80	128.31	120.65
1	A	46	TRP	C-N-CA	5.80	128.31	120.65
2	B	136	VAL	CA-C-N	5.76	127.94	120.56
2	B	136	VAL	C-N-CA	5.76	127.94	120.56
1	A	36	TYR	N-CA-CB	-5.75	102.76	111.21
1	A	50	SER	CA-C-O	5.73	126.55	120.64
1	C	119	THR	CA-CB-OG1	5.68	118.13	109.60
2	B	103	PHE	CA-C-N	5.68	127.89	120.28
2	B	103	PHE	C-N-CA	5.68	127.89	120.28
2	B	24	GLY	CA-C-N	5.66	125.33	119.05
2	B	24	GLY	C-N-CA	5.66	125.33	119.05
1	C	77	LEU	CA-C-N	-5.64	112.41	120.42
1	C	77	LEU	C-N-CA	-5.64	112.41	120.42
2	D	94	ASN	CA-CB-CG	-5.63	106.97	112.60
2	D	77	ASN	CB-CA-C	-5.62	101.67	111.23
2	B	146	PHE	CA-CB-CG	-5.60	108.20	113.80
2	B	7	GLU	CA-C-N	5.59	128.33	120.28
2	B	7	GLU	C-N-CA	5.59	128.33	120.28
2	D	97	PHE	CA-CB-CG	-5.56	108.24	113.80
1	C	54	GLY	CA-C-N	5.54	125.07	119.19
1	C	54	GLY	C-N-CA	5.54	125.07	119.19
1	A	1	SER	N-CA-CB	5.54	119.92	110.50
2	B	57	ASN	CA-C-O	5.54	124.69	119.76
2	D	77	ASN	OD1-CG-ND2	5.54	128.13	122.60
1	A	44	SER	N-CA-C	5.53	119.13	112.38
2	D	135	LYS	N-CA-CB	5.52	118.84	110.28
2	D	143	SER	N-CA-C	5.51	119.26	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	46	TRP	O-C-N	5.51	129.43	123.10
1	A	112	ILE	N-CA-CB	5.49	116.61	110.51
1	A	54	GLY	CA-C-N	5.48	125.00	119.19
1	A	54	GLY	C-N-CA	5.48	125.00	119.19
2	D	35	TYR	CA-C-N	5.47	125.14	119.56
2	D	35	TYR	C-N-CA	5.47	125.14	119.56
2	B	57	ASN	CA-C-N	5.46	125.94	120.04
2	B	57	ASN	C-N-CA	5.46	125.94	120.04
1	A	106	ILE	N-CA-C	-5.43	105.23	110.72
1	A	113	HIS	CA-CB-CG	-5.43	108.37	113.80
2	B	130	TRP	O-C-N	-5.42	116.37	122.12
2	D	44	SER	CA-C-N	5.41	129.34	120.63
2	D	44	SER	C-N-CA	5.41	129.34	120.63
2	D	26	LEU	CA-C-N	5.39	127.45	120.44
2	D	26	LEU	C-N-CA	5.39	127.45	120.44
1	C	1	SER	N-CA-CB	5.38	119.65	110.50
1	A	90	PHE	CA-CB-CG	-5.38	108.42	113.80
1	C	133	VAL	CA-C-N	5.38	127.43	120.44
1	C	133	VAL	C-N-CA	5.38	127.43	120.44
2	B	18	VAL	N-CA-C	5.37	115.83	107.99
2	D	110	LEU	CA-CB-CG	5.36	135.07	116.30
1	C	95	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	59	HIS	CA-CB-CG	-5.34	108.46	113.80
2	B	80	ASN	CA-CB-CG	-5.32	107.28	112.60
1	C	37	PRO	N-CA-C	5.30	120.55	114.03
2	B	51	PRO	N-CA-CB	5.29	109.37	103.44
2	D	50	THR	CA-C-N	5.29	124.92	119.05
2	D	50	THR	C-N-CA	5.29	124.92	119.05
2	D	51	PRO	N-CA-C	-5.29	106.17	113.53
1	A	120	PRO	O-C-N	-5.28	116.48	122.18
1	C	100	LYS	CB-CA-C	-5.28	102.03	110.79
1	A	139	ASP	CA-C-O	-5.28	114.96	120.55
2	B	48	VAL	CA-C-O	5.27	125.63	119.89
1	A	119	THR	CA-C-N	5.25	124.70	119.24
1	A	119	THR	C-N-CA	5.25	124.70	119.24
1	C	139	ASP	CA-C-O	-5.21	114.89	120.42
1	C	49	LEU	CA-C-O	5.21	126.25	119.95
2	B	136	VAL	CA-C-O	5.21	125.87	120.25
2	D	33	ILE	CA-C-O	-5.20	114.48	120.83
2	D	67	VAL	O-C-N	-5.20	116.83	121.87
1	A	13	PHE	CA-C-O	5.18	126.05	120.55
2	D	61	ALA	CA-C-N	5.17	127.21	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	61	ALA	C-N-CA	5.17	127.21	120.28
2	D	143	SER	CA-CB-OG	5.16	121.42	111.10
2	D	62	ALA	N-CA-C	5.16	116.90	111.28
2	D	51	PRO	N-CA-CB	5.14	108.98	103.33
2	B	74	ALA	N-CA-C	-5.09	105.64	111.14
1	C	120	PRO	N-CA-CB	5.09	108.93	103.33
2	B	59	LYS	N-CA-C	-5.09	106.23	112.90
2	B	131	GLN	OE1-CD-NE2	5.08	127.68	122.60
1	A	97	GLY	CA-C-O	5.08	127.44	119.31
2	B	63	HIS	CA-CB-CG	-5.06	108.74	113.80
2	B	48	VAL	N-CA-C	-5.04	107.55	112.29
1	C	38	GLN	OE1-CD-NE2	-5.03	117.57	122.60
2	B	87	SER	CA-C-O	5.02	125.15	119.27
2	D	94	ASN	CA-C-N	-5.02	112.90	122.53
2	D	94	ASN	C-N-CA	-5.02	112.90	122.53

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	1066	0	1092	34	0
1	C	1066	0	1092	38	0
2	B	1121	0	1141	50	0
2	D	1121	0	1141	44	0
3	A	43	0	30	5	0
3	B	43	0	30	5	0
3	C	43	0	30	4	0
3	D	43	0	30	3	0
4	A	2	0	0	2	0
4	B	2	0	0	0	0
4	C	2	0	0	2	0
4	D	2	0	0	0	0
5	A	52	0	0	1	0
5	B	29	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	50	0	0	2	0
5	D	32	0	0	0	0
All	All	4717	0	4586	164	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 18.

All (164) 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:D:1:VAL:HG22	2:D:2:GLU:H	1.39	0.88
2:D:70:ALA:HA	2:D:73:LYS:HE3	1.65	0.79
2:D:92:HIS:HA	2:D:96:LEU:HD12	1.65	0.79
2:D:50:THR:HB	2:D:51:PRO:HD2	1.67	0.75
2:B:20:ILE:HG23	2:B:68:CYS:HB2	1.71	0.72
2:B:132:LYS:O	2:B:136:VAL:HG23	1.88	0.72
2:B:20:ILE:H	2:B:20:ILE:HD12	1.54	0.71
1:A:58:LYS:HE2	1:A:59:HIS:N	2.04	0.71
2:D:1:VAL:HG22	2:D:2:GLU:N	2.06	0.71
1:A:48:ASP:HB3	1:A:53:SER:HB2	1.73	0.70
1:A:59:HIS:HE2	4:A:144:CMO:C	2.04	0.70
2:B:48:VAL:HG13	2:B:54:ILE:HG12	1.74	0.70
2:D:20:ILE:HG13	2:D:68:CYS:HB3	1.74	0.70
3:B:148:HEM:HMC2	3:B:148:HEM:HBC2	1.76	0.68
2:D:50:THR:H	2:D:53:ALA:HB3	1.59	0.67
2:D:73:LYS:O	2:D:77:ASN:HB2	1.95	0.67
2:D:87:SER:O	2:D:91:THR:HG23	1.94	0.67
2:B:1:VAL:HG11	2:B:132:LYS:HE2	1.76	0.66
1:A:7:LYS:O	1:A:11:LYS:HG3	1.97	0.64
2:B:106:LEU:HD22	3:B:148:HEM:CBB	2.26	0.64
2:D:71:LEU:O	2:D:75:VAL:HG23	1.97	0.64
1:C:58:LYS:HE2	1:C:59:HIS:N	2.13	0.64
1:C:7:LYS:O	1:C:11:LYS:HG3	1.99	0.63
1:A:85:SER:HB3	1:A:140:LYS:HG2	1.81	0.63
3:A:143:HEM:HMC2	3:A:143:HEM:HBC2	1.81	0.63
3:D:148:HEM:HBC2	3:D:148:HEM:HMC2	1.81	0.62
1:A:48:ASP:HB3	1:A:53:SER:CB	2.30	0.61
1:C:111:ALA:HB1	2:D:116:ALA:HB2	1.81	0.61
2:D:50:THR:HB	2:D:51:PRO:CD	2.30	0.61
2:B:14:VAL:O	2:B:18:VAL:HG23	2.00	0.61
2:B:70:ALA:HA	2:B:73:LYS:NZ	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:PHE:CE2	2:D:1:VAL:HB	2.37	0.60
3:B:148:HEM:HHA	3:B:148:HEM:HBA1	1.84	0.60
2:D:70:ALA:HA	2:D:73:LYS:CE	2.33	0.59
1:A:1:SER:HB2	1:C:139:ASP:OD1	2.02	0.59
2:B:72:ASP:O	2:B:76:LYS:HD2	2.03	0.59
2:D:1:VAL:CG2	2:D:2:GLU:H	2.13	0.58
1:C:119:THR:HB	1:C:120:PRO:CD	2.33	0.58
1:C:87:LEU:HA	1:C:91:LYS:HE2	1.86	0.58
1:C:119:THR:HB	1:C:120:PRO:HD2	1.85	0.57
1:A:128:LYS:HD2	1:C:142:ARG:HG3	1.87	0.57
3:A:143:HEM:HBC2	3:A:143:HEM:CMC	2.34	0.57
1:C:13:PHE:O	1:C:17:ILE:HG23	2.05	0.57
3:B:148:HEM:HHA	3:B:148:HEM:CBA	2.35	0.57
1:A:50:SER:HB2	1:A:51:PRO:HD2	1.86	0.56
2:B:4:THR:O	2:B:8:LYS:HG3	2.04	0.56
2:B:78:MET:HE3	2:B:133:PHE:CD1	2.40	0.56
1:C:0:ACE:H3	5:C:148:HOH:O	2.05	0.56
2:D:8:LYS:HA	2:D:78:MET:HE1	1.87	0.56
1:C:124:ILE:CD1	2:D:34:VAL:HA	2.35	0.56
2:B:136:VAL:HG22	2:D:146:PHE:CE1	2.41	0.55
1:C:124:ILE:HD13	2:D:34:VAL:HA	1.89	0.55
2:B:73:LYS:O	2:B:77:ASN:HB2	2.07	0.55
2:B:78:MET:HA	2:B:81:ILE:HD11	1.88	0.54
2:D:106:LEU:HD22	3:D:148:HEM:CBB	2.38	0.54
1:C:59:HIS:HE2	4:C:144:CMO:C	2.21	0.53
2:B:107:ALA:CB	2:B:134:MET:HE2	2.39	0.53
1:A:59:HIS:NE2	4:A:144:CMO:O	2.39	0.53
2:D:55:MET:HE3	2:D:55:MET:HA	1.90	0.52
1:C:14:TRP:CZ3	1:C:17:ILE:HD11	2.44	0.52
1:C:106:ILE:O	1:C:110:LEU:HG	2.09	0.52
2:D:47:ASN:O	2:D:53:ALA:HB1	2.10	0.52
1:A:5:LYS:O	1:A:9:VAL:HG23	2.10	0.51
2:D:25:PRO:HB3	2:D:61:ALA:HA	1.92	0.51
1:A:98:ASN:HB3	3:A:143:HEM:HBC2	1.93	0.51
1:C:48:ASP:HB3	1:C:53:SER:HB2	1.92	0.51
2:D:106:LEU:HD22	3:D:148:HEM:HBB2	1.91	0.51
2:B:50:THR:HB	2:B:51:PRO:CD	2.41	0.51
2:B:70:ALA:O	2:B:73:LYS:HG3	2.11	0.50
1:C:84:LEU:HD22	1:C:88:HIS:HE1	1.77	0.50
1:C:102:LEU:HD23	3:C:143:HEM:HAB	1.94	0.50
3:C:143:HEM:HMC1	3:C:143:HEM:HBC2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:ASN:O	2:B:79:GLY:N	2.44	0.49
2:D:82:LEU:HD23	2:D:140:ALA:HA	1.93	0.49
1:C:96:PRO:HG3	1:C:141:TYR:CE2	2.46	0.49
1:A:87:LEU:HD12	1:A:91:LYS:HB2	1.94	0.49
2:B:146:PHE:O	2:D:135:LYS:HE3	2.13	0.49
1:A:46:TRP:HB2	1:A:49:LEU:HD21	1.95	0.49
2:B:107:ALA:HB1	2:B:134:MET:HE2	1.95	0.49
1:A:81:MET:HE2	1:A:133:VAL:HG13	1.95	0.49
1:A:124:ILE:HG12	2:B:34:VAL:HA	1.93	0.49
2:B:1:VAL:HG22	2:B:2:GLU:H	1.76	0.48
2:B:47:ASN:HD22	2:B:53:ALA:HB1	1.78	0.48
1:A:62:ILE:HD12	5:A:160:HOH:O	2.12	0.48
2:B:7:GLU:O	2:B:10:THR:HB	2.14	0.48
1:A:78:VAL:HA	1:A:136:ALA:HB1	1.95	0.48
2:D:8:LYS:HG2	2:D:78:MET:CE	2.44	0.48
1:A:17:ILE:O	1:A:18:SER:C	2.57	0.47
2:D:45:PHE:CD1	2:D:45:PHE:N	2.82	0.47
2:D:78:MET:HA	2:D:81:ILE:HD11	1.94	0.47
1:C:84:LEU:HD22	1:C:88:HIS:CE1	2.49	0.47
1:C:107:LEU:HD22	1:C:118:PHE:HZ	1.79	0.47
2:B:70:ALA:HA	2:B:73:LYS:HZ2	1.79	0.47
1:A:46:TRP:HE3	1:A:49:LEU:HD22	1.80	0.46
1:C:11:LYS:NZ	5:C:193:HOH:O	2.48	0.46
2:B:47:ASN:HD22	2:B:53:ALA:CB	2.28	0.46
3:B:148:HEM:HBA1	3:B:148:HEM:CHA	2.44	0.46
2:D:84:THR:HG22	2:D:85:TYR:HD1	1.79	0.46
2:B:50:THR:HB	2:B:51:PRO:HD2	1.97	0.46
2:D:82:LEU:CD2	2:D:140:ALA:HA	2.46	0.46
2:D:45:PHE:N	2:D:45:PHE:HD1	2.14	0.46
2:D:3:TRP:CH2	2:D:132:LYS:HG2	2.50	0.46
1:C:43:PHE:O	1:C:49:LEU:HD21	2.16	0.46
1:A:99:PHE:HB2	1:A:100:LYS:HE3	1.97	0.45
2:B:70:ALA:HA	2:B:73:LYS:HZ3	1.81	0.45
2:B:134:MET:O	2:B:138:VAL:HG23	2.16	0.45
2:B:50:THR:O	2:B:54:ILE:HG13	2.17	0.45
2:B:82:LEU:HD23	2:B:82:LEU:HA	1.89	0.45
1:A:25:GLY:HA3	1:A:60:GLY:O	2.15	0.45
2:B:99:ASP:OD1	2:B:101:ASP:HB2	2.17	0.45
2:B:123:THR:HB	2:B:124:PRO:HD2	1.99	0.45
1:A:42:TYR:CE1	1:A:94:VAL:HA	2.52	0.45
2:B:55:MET:HE3	2:B:55:MET:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:LEU:HD12	1:C:32:MET:HE2	1.99	0.45
2:B:142:GLY:HA2	2:B:145:TYR:CD1	2.52	0.44
2:D:123:THR:HB	2:D:124:PRO:HD2	1.98	0.44
2:B:82:LEU:HD23	2:B:140:ALA:HA	1.98	0.44
2:B:22:GLU:O	2:B:26:LEU:HG	2.18	0.44
2:B:82:LEU:CD2	2:B:140:ALA:HA	2.47	0.44
1:C:87:LEU:HD12	1:C:91:LYS:HB2	2.00	0.44
2:D:86:LYS:HD3	2:D:86:LYS:HA	1.71	0.44
1:C:54:GLY:N	1:C:55:PRO:CD	2.80	0.43
1:C:81:MET:HE2	1:C:133:VAL:HG13	2.00	0.43
2:D:25:PRO:HG3	2:D:61:ALA:O	2.18	0.43
1:C:68:GLY:O	1:C:71:VAL:HB	2.17	0.43
2:B:5:ASP:HA	2:B:8:LYS:HE2	2.01	0.43
1:A:102:LEU:HD23	3:A:143:HEM:HAB	2.01	0.43
2:B:77:ASN:OD1	2:B:80:ASN:HB2	2.18	0.43
2:B:1:VAL:HG22	2:B:2:GLU:N	2.34	0.43
1:A:32:MET:O	1:A:36:TYR:HB2	2.19	0.43
1:A:54:GLY:N	1:A:55:PRO:HD2	2.34	0.43
1:C:91:LYS:N	1:C:91:LYS:HD3	2.33	0.42
2:D:8:LYS:HG2	2:D:78:MET:HE2	2.00	0.42
3:C:143:HEM:HBC2	3:C:143:HEM:CMC	2.49	0.42
2:D:107:ALA:HA	2:D:134:MET:HE2	2.01	0.42
1:A:94:VAL:HG12	1:A:95:ASP:O	2.20	0.42
1:A:139:ASP:OD1	1:C:1:SER:HB2	2.19	0.42
2:B:80:ASN:HB3	2:B:83:ALA:HB3	2.02	0.42
1:C:124:ILE:HG12	2:D:34:VAL:HG22	2.01	0.42
3:A:143:HEM:HHA	3:A:143:HEM:HBD2	2.01	0.42
2:D:57:ASN:HA	2:D:58:PRO:HD3	1.66	0.42
2:B:82:LEU:HD22	2:B:86:LYS:HE2	2.01	0.42
1:C:59:HIS:NE2	4:C:144:CMO:O	2.45	0.42
2:D:92:HIS:CA	2:D:96:LEU:HD12	2.43	0.42
1:A:71:VAL:O	1:A:74:MET:HE2	2.20	0.41
2:B:87:SER:HA	2:B:90:GLU:HB2	2.02	0.41
1:A:6:ASP:O	1:A:10:VAL:HG23	2.20	0.41
2:B:86:LYS:HD3	2:B:86:LYS:HA	1.65	0.41
1:C:50:SER:HA	1:C:51:PRO:HD3	1.93	0.41
2:B:47:ASN:O	2:B:53:ALA:HB1	2.21	0.41
1:C:46:TRP:HB2	1:C:49:LEU:HD21	2.01	0.41
2:B:87:SER:O	2:B:91:THR:HG23	2.21	0.41
2:B:91:THR:HG21	5:B:154:HOH:O	2.20	0.41
1:A:68:GLY:O	1:A:71:VAL:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ARG:HB3	2:D:36:PRO:HG2	2.02	0.41
1:C:95:ASP:HA	1:C:96:PRO:HD3	1.87	0.41
1:A:54:GLY:N	1:A:55:PRO:CD	2.84	0.41
2:D:82:LEU:HD23	2:D:82:LEU:HA	1.91	0.41
2:D:84:THR:HG22	2:D:85:TYR:CD1	2.55	0.41
1:C:107:LEU:HD22	1:C:118:PHE:CZ	2.56	0.41
2:B:37:TRP:O	2:B:40:ARG:HG2	2.21	0.41
1:C:102:LEU:HD23	3:C:143:HEM:CAB	2.51	0.41
1:A:13:PHE:HA	1:A:16:LYS:HG3	2.02	0.40
1:C:58:LYS:HE2	1:C:59:HIS:CA	2.51	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	141/143 (99%)	136 (96%)	4 (3%)	1 (1%)	18	34
1	C	141/143 (99%)	137 (97%)	3 (2%)	1 (1%)	18	34
2	B	144/146 (99%)	139 (96%)	4 (3%)	1 (1%)	18	34
2	D	144/146 (99%)	138 (96%)	5 (4%)	1 (1%)	18	34
All	All	570/578 (99%)	550 (96%)	16 (3%)	4 (1%)	18	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	78	MET
1	C	1	SER
1	A	1	SER
2	D	78	MET

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	110/110 (100%)	99 (90%)	11 (10%)	7	15
1	C	110/110 (100%)	99 (90%)	11 (10%)	7	15
2	B	117/117 (100%)	95 (81%)	22 (19%)	1	3
2	D	117/117 (100%)	103 (88%)	14 (12%)	5	10
All	All	454/454 (100%)	396 (87%)	58 (13%)	4	9

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	16	LYS
1	A	18	SER
1	A	20	LYS
1	A	49	LEU
1	A	58	LYS
1	A	84	LEU
1	A	100	LYS
1	A	124	ILE
1	A	130	LEU
1	A	140	LYS
2	B	2	GLU
2	B	7	GLU
2	B	10	THR
2	B	12	SER
2	B	17	LYS
2	B	23	ILE
2	B	40	ARG
2	B	49	SER
2	B	71	LEU
2	B	73	LYS
2	B	76	LYS
2	B	77	ASN
2	B	86	LYS

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Mol	Chain	Res	Type
2	B	87	SER
2	B	88	LEU
2	B	95	LYS
2	B	105	VAL
2	B	110	LEU
2	B	117	LYS
2	B	121	SER
2	B	129	THR
2	B	131	GLN
1	C	5	LYS
1	C	16	LYS
1	C	20	LYS
1	C	44	SER
1	C	58	LYS
1	C	78	VAL
1	C	100	LYS
1	C	116	SER
1	C	122	VAL
1	C	124	ILE
1	C	130	LEU
2	D	2	GLU
2	D	9	SER
2	D	17	LYS
2	D	40	ARG
2	D	48	VAL
2	D	71	LEU
2	D	76	LYS
2	D	87	SER
2	D	95	LYS
2	D	104	ARG
2	D	110	LEU
2	D	117	LYS
2	D	129	THR
2	D	144	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	105	ASN
2	B	47	ASN
1	C	38	GLN

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Mol	Chain	Res	Type
2	D	102	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](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	HEM	D	148	2	50,50,50	1.27	7 (14%)	67,82,82	1.28	4 (5%)
3	HEM	B	148	2	50,50,50	1.33	8 (16%)	67,82,82	0.99	4 (5%)
3	HEM	A	143	1	50,50,50	1.22	5 (10%)	67,82,82	1.15	5 (7%)
4	CMO	C	144	-	0,1,1	-	-	-	-	-
3	HEM	C	143	1	50,50,50	1.25	9 (18%)	67,82,82	1.28	7 (10%)
4	CMO	D	149	-	0,1,1	-	-	-	-	-
4	CMO	A	144	-	0,1,1	-	-	-	-	-
4	CMO	B	149	-	0,1,1	-	-	-	-	-

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	A	143	1	-	5/14/54/54	-
3	HEM	D	148	2	-	4/14/54/54	-
3	HEM	C	143	1	-	4/14/54/54	-
3	HEM	B	148	2	-	6/14/54/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	148	HEM	CAB-C3B	3.15	1.55	1.47
3	B	148	HEM	CAC-C3C	2.99	1.55	1.47
3	D	148	HEM	FE-NB	2.94	2.03	1.94
3	B	148	HEM	FE-NB	2.68	2.03	1.94
3	C	143	HEM	CAB-C3B	2.68	1.54	1.47
3	A	143	HEM	CAB-C3B	2.65	1.54	1.47
3	D	148	HEM	CAC-C3C	2.64	1.54	1.47
3	D	148	HEM	FE-NC	2.64	2.03	1.95
3	B	148	HEM	CMB-C2B	2.63	1.56	1.50
3	B	148	HEM	FE-NC	2.63	2.03	1.95
3	D	148	HEM	CMB-C2B	2.61	1.56	1.50
3	A	143	HEM	FE-ND	2.49	2.02	1.94
3	C	143	HEM	FE-ND	2.47	2.02	1.94
3	B	148	HEM	CAB-C3B	2.44	1.53	1.47
3	A	143	HEM	FE-NC	2.41	2.03	1.95
3	C	143	HEM	CAC-C3C	2.35	1.53	1.47
3	A	143	HEM	FE-NB	2.33	2.02	1.94
3	C	143	HEM	CMB-C2B	2.30	1.55	1.50
3	A	143	HEM	CMB-C2B	2.27	1.55	1.50
3	B	148	HEM	FE-NA	2.26	2.02	1.95
3	D	148	HEM	CMA-C3A	2.23	1.55	1.50
3	D	148	HEM	C2A-C3A	-2.19	1.33	1.38
3	C	143	HEM	CMD-C2D	2.19	1.55	1.50
3	C	143	HEM	FE-NB	2.18	2.01	1.94
3	C	143	HEM	C2A-C3A	-2.11	1.33	1.38
3	C	143	HEM	FE-NA	2.11	2.02	1.95
3	B	148	HEM	C2A-C3A	-2.04	1.33	1.38
3	C	143	HEM	O1D-CGD	2.01	1.28	1.22
3	B	148	HEM	CMC-C2C	2.01	1.54	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	148	HEM	CAA-CBA-CGA	4.24	124.91	113.67
3	C	143	HEM	CMA-C3A-C4A	-3.99	119.34	125.42
3	D	148	HEM	CMA-C3A-C4A	-3.82	119.61	125.42
3	A	143	HEM	CMA-C3A-C2A	3.62	133.30	125.62
3	A	143	HEM	CMA-C3A-C4A	-3.55	120.01	125.42
3	C	143	HEM	CMA-C3A-C2A	3.45	132.94	125.62
3	C	143	HEM	CHB-C4A-NA	3.37	129.98	123.86
3	D	148	HEM	CMA-C3A-C2A	2.96	131.90	125.62
3	B	148	HEM	O1A-CGA-CBA	-2.40	115.48	123.09
3	C	143	HEM	C4A-CHB-C1B	-2.39	120.64	126.25
3	B	148	HEM	CMA-C3A-C2A	2.33	130.56	125.62
3	C	143	HEM	C3B-C2B-C1B	2.27	108.11	106.41
3	A	143	HEM	O2A-CGA-O1A	2.26	129.15	123.33
3	C	143	HEM	CHB-C1B-NB	2.21	127.10	124.37
3	B	148	HEM	CBB-CAB-C3B	-2.21	116.50	127.53
3	A	143	HEM	O1D-CGD-CBD	-2.16	116.23	123.09
3	C	143	HEM	CAD-CBD-CGD	2.13	119.31	113.67
3	D	148	HEM	CHB-C4A-NA	2.12	127.71	123.86
3	A	143	HEM	CHB-C4A-NA	2.10	127.67	123.86
3	B	148	HEM	CMA-C3A-C4A	-2.01	122.35	125.42

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	148	HEM	C1A-C2A-CAA-CBA
3	B	148	HEM	C3A-C2A-CAA-CBA
3	B	148	HEM	C3D-CAD-CBD-CGD
3	D	148	HEM	C2B-C3B-CAB-CBB
3	D	148	HEM	C4B-C3B-CAB-CBB
3	B	148	HEM	C2A-CAA-CBA-CGA
3	D	148	HEM	C2A-CAA-CBA-CGA
3	D	148	HEM	C3D-CAD-CBD-CGD
3	A	143	HEM	C4D-C3D-CAD-CBD
3	B	148	HEM	C2B-C3B-CAB-CBB
3	B	148	HEM	C4B-C3B-CAB-CBB
3	A	143	HEM	C3D-CAD-CBD-CGD
3	A	143	HEM	C2D-C3D-CAD-CBD
3	C	143	HEM	CAD-CBD-CGD-O2D
3	C	143	HEM	CAD-CBD-CGD-O1D
3	A	143	HEM	CAD-CBD-CGD-O1D
3	A	143	HEM	CAD-CBD-CGD-O2D
3	C	143	HEM	CAA-CBA-CGA-O2A

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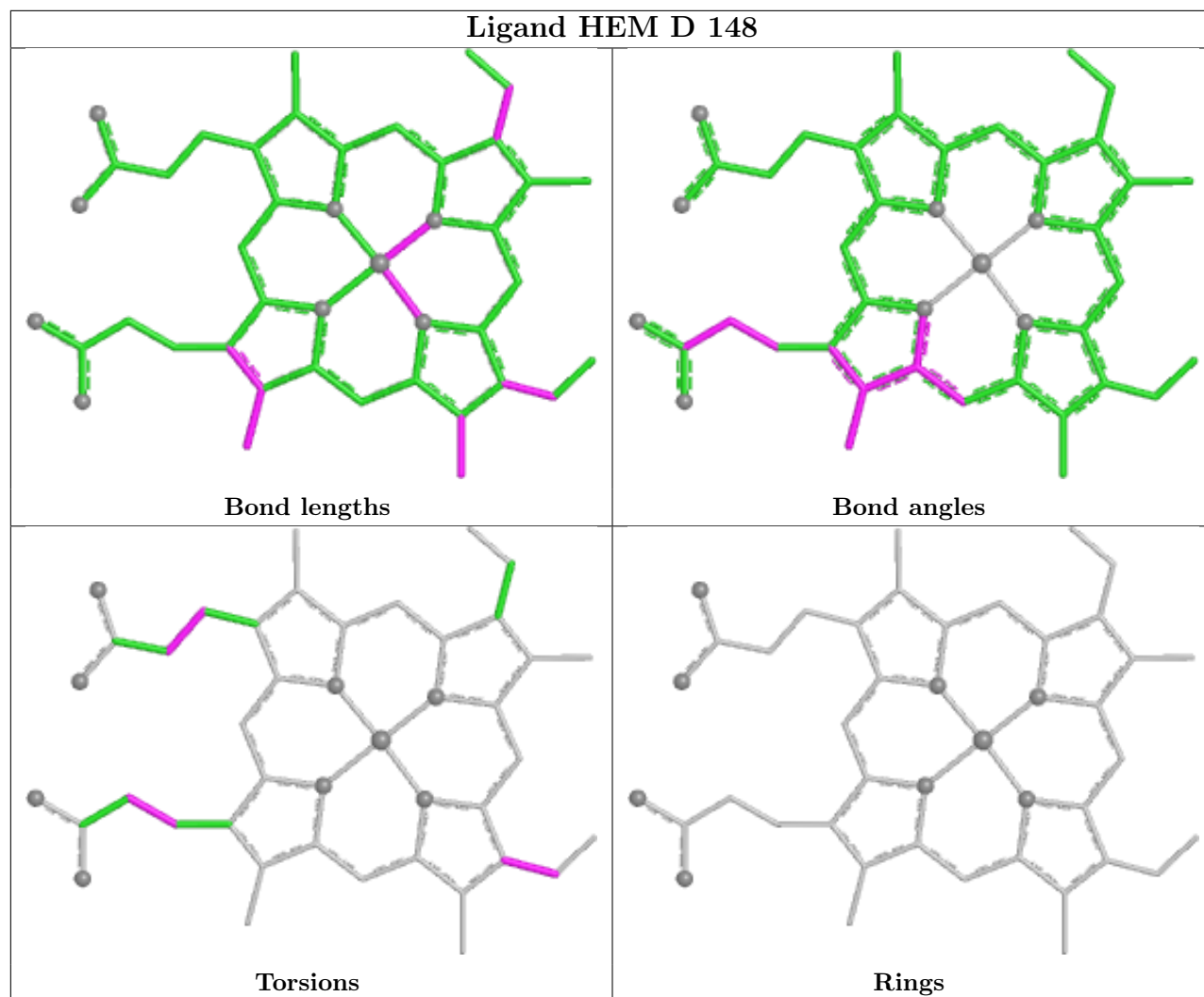
Mol	Chain	Res	Type	Atoms
3	C	143	HEM	CAA-CBA-CGA-O1A

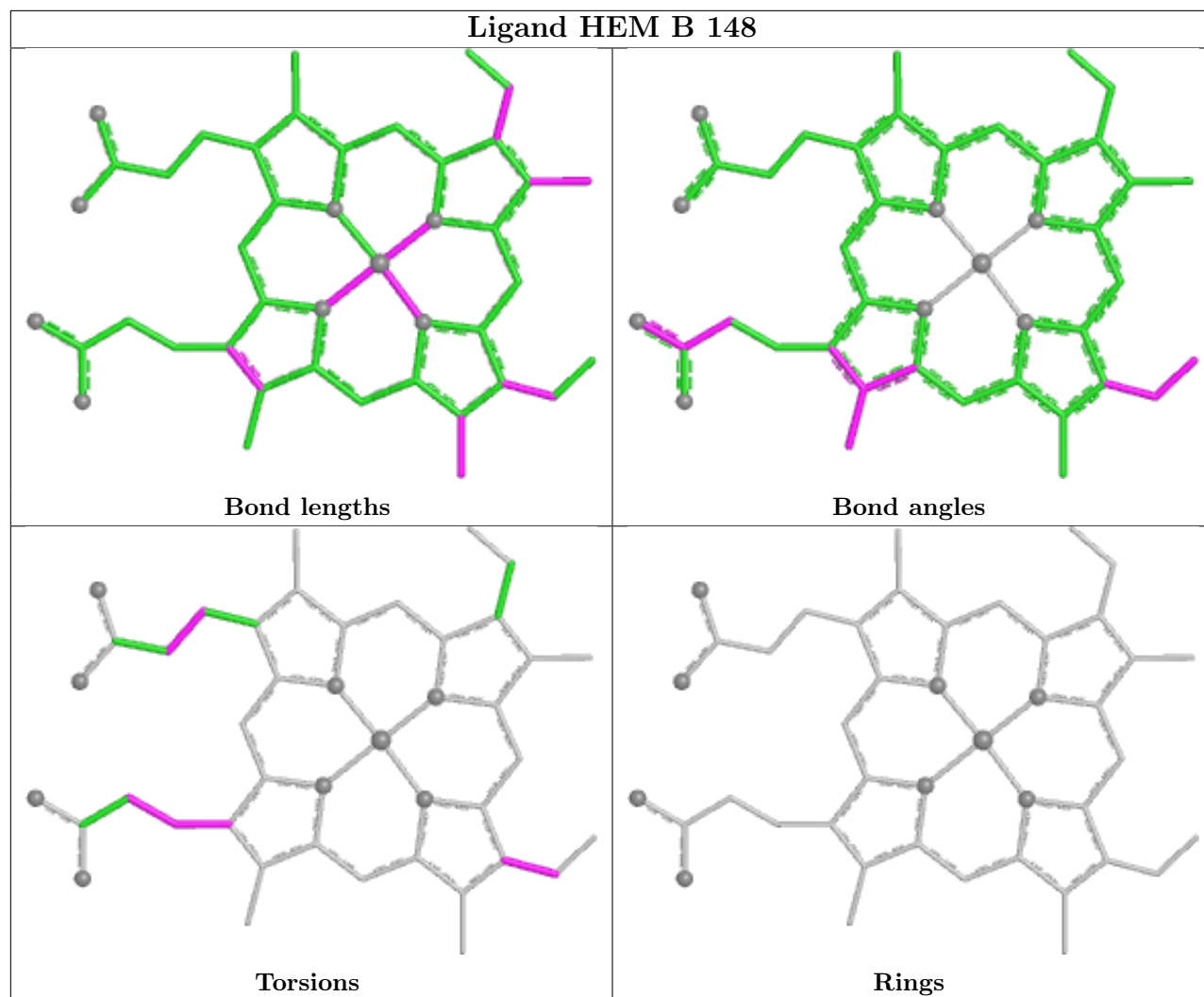
There are no ring outliers.

6 monomers are involved in 21 short contacts:

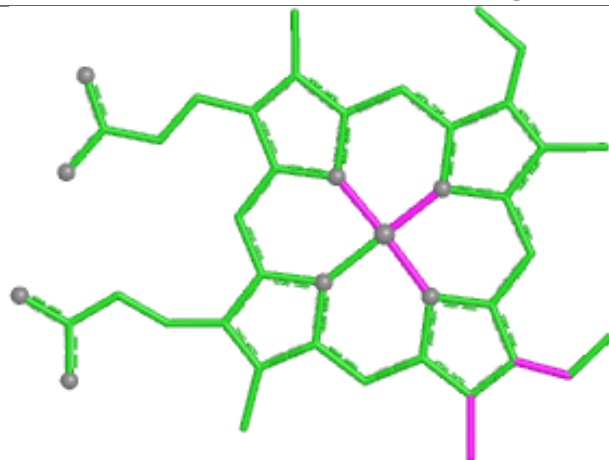
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	148	HEM	3	0
3	B	148	HEM	5	0
3	A	143	HEM	5	0
4	C	144	CMO	2	0
3	C	143	HEM	4	0
4	A	144	CMO	2	0

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.

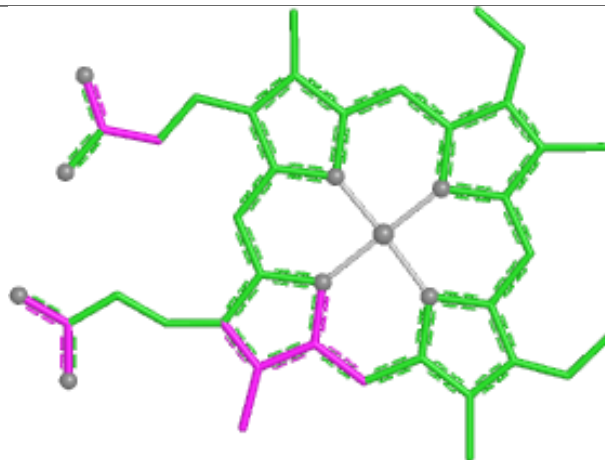




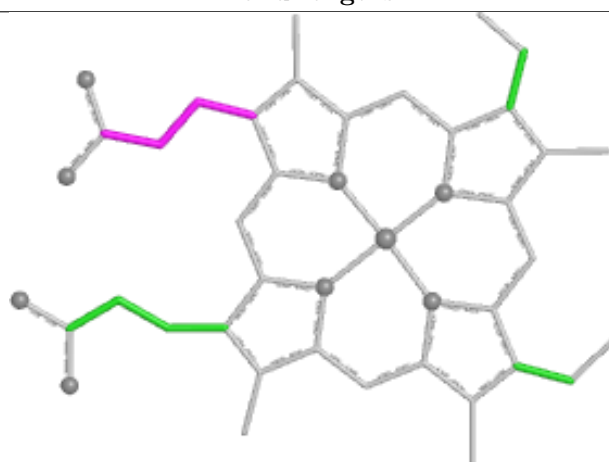
Ligand HEM A 143



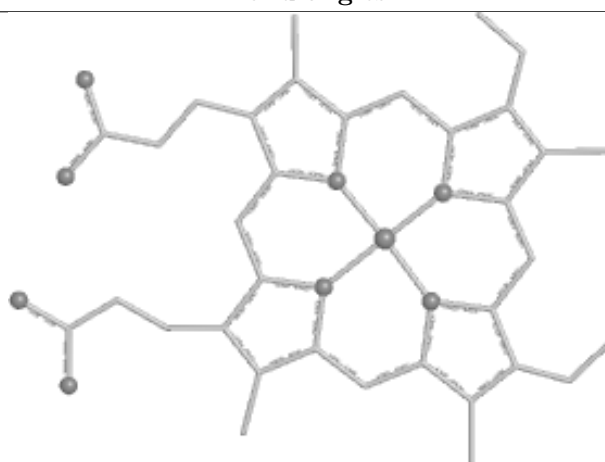
Bond lengths



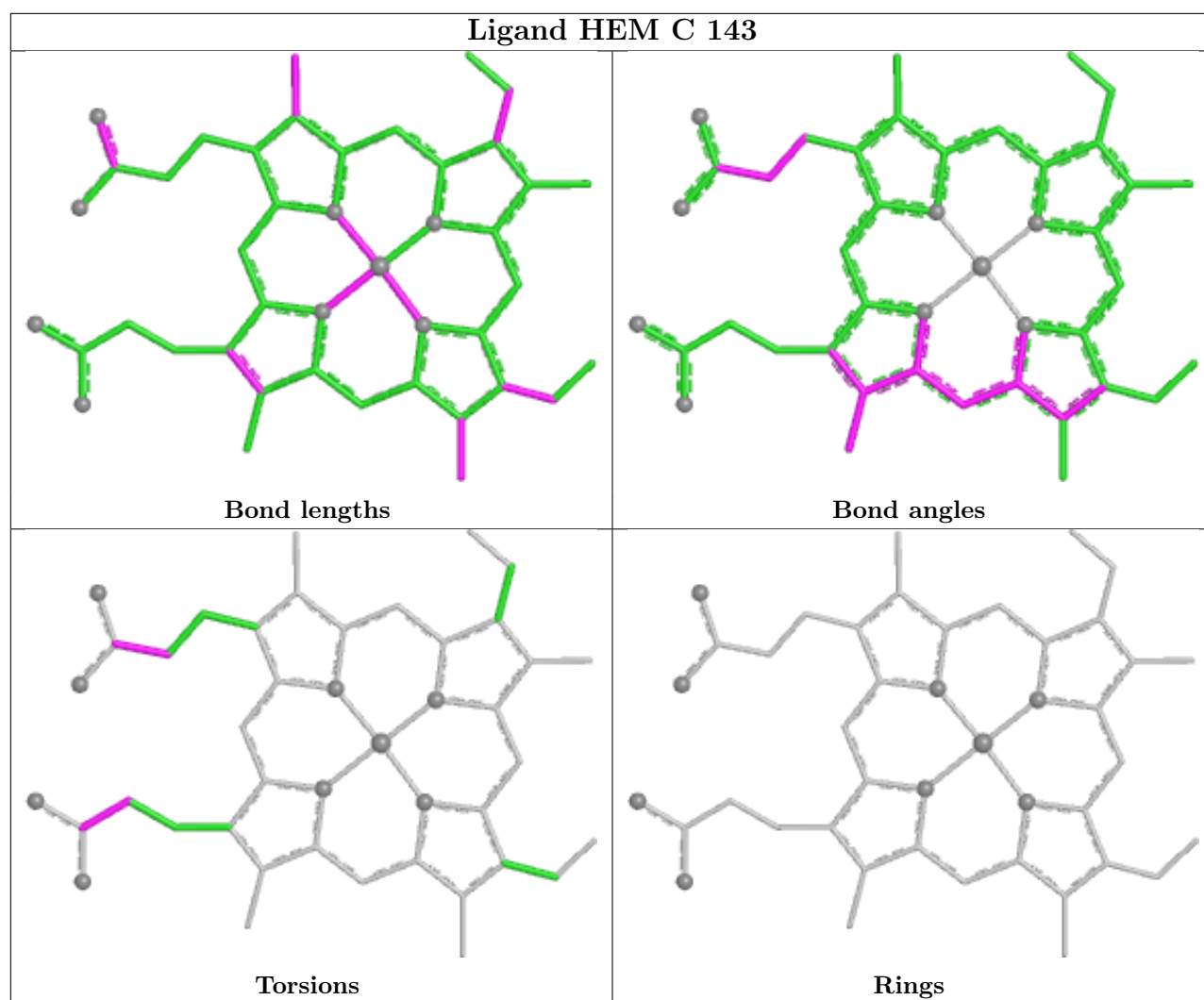
Bond angles



Torsions



Rings



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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.