



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:02 PM UTC

PDB ID : 1DKE / pdb_00001dke
Title : NI BETA HEME HUMAN HEMOGLOBIN
Authors : Bruno, S.; Bettatti, S.; Mozzarelli, A.; Bolognesi, M.; Deriu, D.; Rosano, C.;
Tsuneshige, A.; Yonetani, T.; Henry, E.R.
Deposited on : 1999-12-07
Resolution : 2.10 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) : 2.49

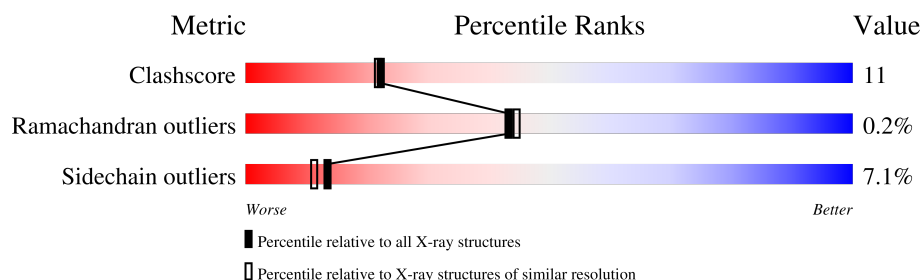
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	141	
1	C	141	
2	B	146	
2	D	146	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4823 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.

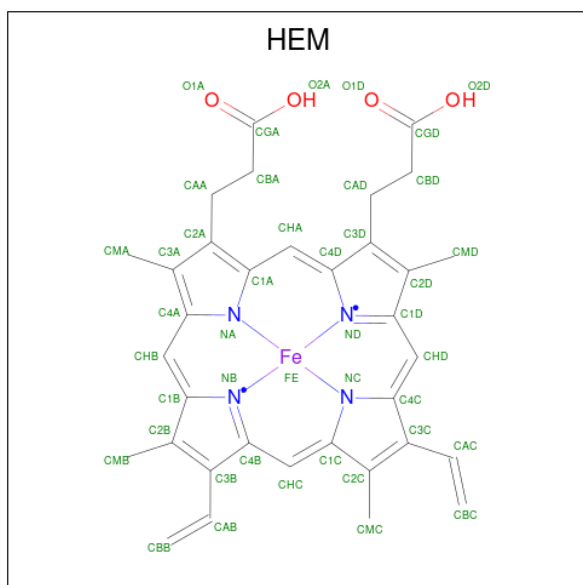
- Molecule 1 is a protein called HEMOGLOBIN: ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1068	685	187	193	3			
1	C	141	Total	C	N	O	S	11	0	0
			1068	685	187	193	3			

- Molecule 2 is a protein called HEMOGLOBIN: BETA CHAIN.

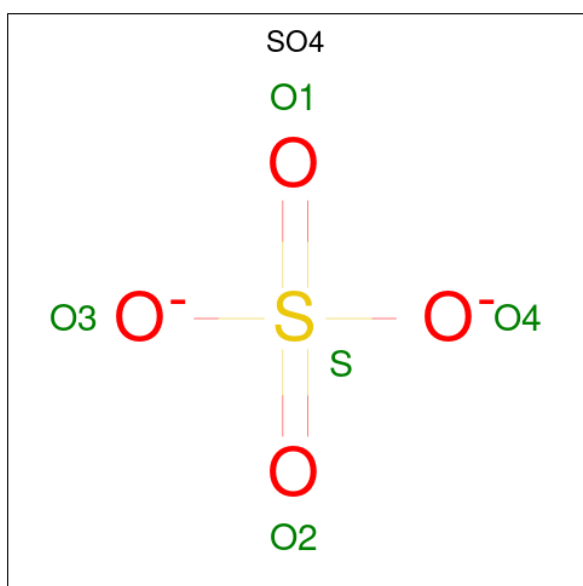
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	19	0	0
			1122	724	195	200	3			
2	D	146	Total	C	N	O	S	18	0	0
			1122	724	195	200	3			

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O S		
			5	4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	74	Total	O		
			74	74	0	0
5	B	88	Total	O		
			88	88	0	0
5	C	57	Total	O		
			57	57	0	0
5	D	47	Total	O		
			47	47	0	0

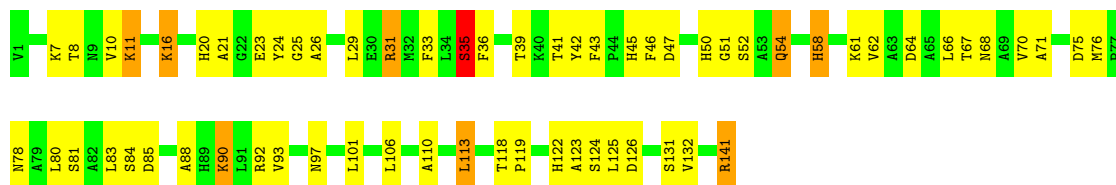
3 Residue-property plots

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.

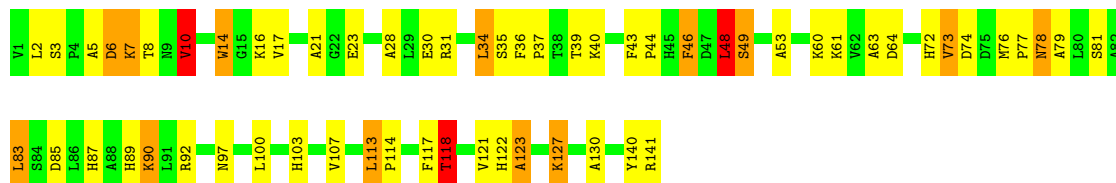
• Molecule 1: HEMOGLOBIN: ALPHA CHAIN

Chain A: 



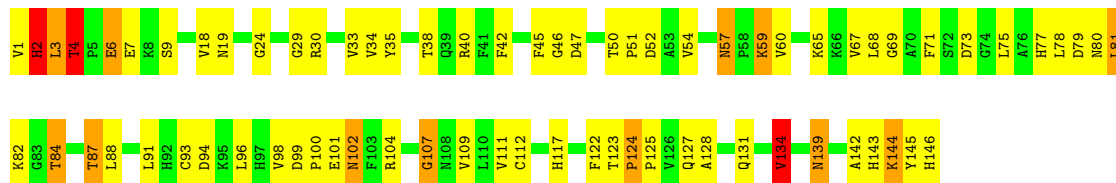
• Molecule 1: HEMOGLOBIN: ALPHA CHAIN

Chain C: 



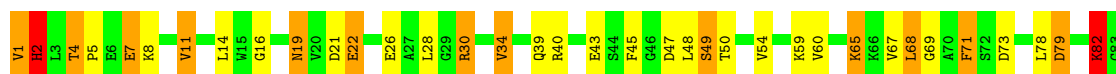
• Molecule 2: HEMOGLOBIN: BETA CHAIN

Chain B: 



• Molecule 2: HEMOGLOBIN: BETA CHAIN

Chain D: 



T84	F85	A86	T87	E90	L91	H92	C93	D94	E101	M102	F103	R104	N108	V109	L110	V111	C112	V113	H116	H117	F118	E121	F122	T123	P124	P125	V126	Q127	Y130	Q131	K132	V133	V134	A135	A138	M139	A140	H143	H146
-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.72Å 81.40Å 63.15Å 90.00° 97.81° 90.00°	Depositor
Resolution (Å)	12.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4823	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, SO4

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	1.27	0/1096	2.46	75/1491 (5.0%)
1	C	1.21	0/1096	2.45	75/1491 (5.0%)
2	B	1.72	8/1152 (0.7%)	2.52	81/1566 (5.2%)
2	D	1.22	4/1152 (0.3%)	2.61	79/1566 (5.0%)
All	All	1.38	12/4496 (0.3%)	2.51	310/6114 (5.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	1	0
2	B	1	0
2	D	1	2
All	All	3	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	VAL	C-N	35.33	1.82	1.33
2	D	1	VAL	C-N	14.83	1.54	1.33
2	B	3	LEU	CB-CG	14.67	1.82	1.53
2	B	144	LYS	CD-CE	-7.69	1.29	1.52
2	B	144	LYS	CG-CD	7.49	1.75	1.52
2	B	78	LEU	CG-CD1	6.15	1.72	1.52
2	D	2	HIS	CA-CB	5.52	1.62	1.53
2	B	145	TYR	N-CA	5.45	1.53	1.45
2	B	99	ASP	N-CA	5.24	1.53	1.46
2	D	146	HIS	C-O	5.21	1.33	1.23
2	D	69	GLY	N-CA	5.12	1.52	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	65	LYS	CG-CD	5.01	1.67	1.52

All (310) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	VAL	O-C-N	-39.92	59.13	123.00
2	B	1	VAL	CA-C-N	-15.73	98.55	121.99
2	B	1	VAL	C-N-CA	-15.73	98.55	121.99
1	A	92	ARG	CD-NE-CZ	13.14	142.80	124.40
2	B	134	VAL	N-CA-CB	13.03	128.26	110.54
1	A	75	ASP	CA-CB-CG	12.04	124.64	112.60
1	A	141	ARG	CA-C-O	-11.89	100.59	120.80
2	B	47	ASP	CA-CB-CG	11.35	123.95	112.60
2	D	146	HIS	CA-C-O	-11.22	101.73	120.80
1	A	33	PHE	CA-CB-CG	10.72	124.52	113.80
1	C	141	ARG	CA-C-O	-10.43	103.07	120.80
2	D	71	PHE	CA-CB-CG	10.33	124.13	113.80
1	C	117	PHE	O-C-N	-10.14	109.22	122.61
2	D	124	PRO	CB-CA-C	10.00	123.12	110.92
2	B	71	PHE	CA-CB-CG	9.88	123.68	113.80
1	C	118	THR	N-CA-CB	-9.75	96.88	109.55
1	C	2	LEU	CA-C-O	-9.73	109.96	121.05
1	C	122	HIS	CA-CB-CG	9.57	123.37	113.80
1	A	122	HIS	CA-CB-CG	9.50	123.30	113.80
2	B	2	HIS	CA-C-O	9.48	131.31	120.60
2	B	4	THR	N-CA-CB	-9.47	96.71	109.78
1	A	61	LYS	CA-C-O	-9.42	110.93	120.82
2	D	143	HIS	N-CA-C	9.41	122.40	111.11
2	B	104	ARG	NE-CZ-NH1	-9.36	112.14	121.50
1	A	61	LYS	O-C-N	9.31	131.66	122.07
1	C	117	PHE	CA-C-O	9.21	134.79	122.44
1	C	10	VAL	N-CA-C	9.17	119.22	110.42
1	C	31	ARG	NE-CZ-NH2	-9.15	110.96	119.20
2	D	47	ASP	CA-CB-CG	9.11	121.71	112.60
2	B	134	VAL	CA-CB-CG1	9.05	125.79	110.40
2	D	60	VAL	N-CA-CB	9.03	121.11	110.55
2	B	146	HIS	CA-C-O	-8.80	105.83	120.80
1	A	50	HIS	CA-C-O	-8.80	110.89	120.92
1	A	62	VAL	N-CA-CB	8.45	119.89	110.51
2	B	54	VAL	O-C-N	8.44	130.68	121.90
1	A	51	GLY	CA-C-O	8.44	128.51	119.06
2	D	2	HIS	CA-CB-CG	8.43	122.23	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	7	LYS	CA-C-O	-8.40	111.64	120.55
1	C	103	HIS	CA-CB-CG	8.35	122.15	113.80
2	D	104	ARG	NE-CZ-NH2	8.31	126.68	119.20
2	D	93	CYS	CA-C-N	8.22	131.12	120.44
2	D	93	CYS	C-N-CA	8.22	131.12	120.44
1	C	127	LYS	N-CA-CB	8.19	122.16	110.12
1	C	6	ASP	CA-C-O	8.16	129.63	120.90
2	B	99	ASP	CA-C-N	8.10	127.75	119.82
2	B	99	ASP	C-N-CA	8.10	127.75	119.82
2	D	79	ASP	CA-CB-CG	-8.04	104.56	112.60
2	D	103	PHE	CA-CB-CG	8.03	121.83	113.80
1	A	67	THR	O-C-N	7.94	130.53	122.12
2	D	30	ARG	NE-CZ-NH2	7.85	126.26	119.20
1	C	81	SER	N-CA-CB	7.78	121.68	110.16
2	D	1	VAL	CA-C-N	-7.74	106.76	121.54
2	D	1	VAL	C-N-CA	-7.74	106.76	121.54
1	C	36	PHE	N-CA-CB	-7.70	99.89	111.21
1	A	21	ALA	CA-C-N	7.70	128.52	119.98
1	A	21	ALA	C-N-CA	7.70	128.52	119.98
1	A	23	GLU	CA-CB-CG	7.67	129.43	114.10
1	C	8	THR	CA-CB-OG1	-7.59	98.21	109.60
2	D	116	HIS	O-C-N	7.57	129.87	122.07
1	C	140	TYR	N-CA-C	7.49	119.44	111.28
2	B	104	ARG	NE-CZ-NH2	7.47	125.92	119.20
2	B	9	SER	CA-C-O	7.46	129.28	120.92
2	B	35	TYR	CA-C-N	7.45	127.16	119.56
2	B	35	TYR	C-N-CA	7.45	127.16	119.56
2	B	139	ASN	CA-CB-CG	7.43	120.03	112.60
2	B	18	VAL	N-CA-C	7.40	119.56	108.23
1	C	7	LYS	O-C-N	7.39	129.96	122.12
2	B	19	ASN	CA-C-N	7.39	130.95	120.53
2	B	19	ASN	C-N-CA	7.39	130.95	120.53
2	B	73	ASP	CA-CB-CG	-7.36	105.25	112.60
1	C	48	LEU	N-CA-C	7.34	121.89	113.15
1	C	36	PHE	CA-C-N	7.32	127.96	119.47
1	C	36	PHE	C-N-CA	7.32	127.96	119.47
1	A	25	GLY	O-C-N	-7.31	115.17	122.19
1	A	70	VAL	N-CA-CB	7.30	120.47	110.54
2	D	126	VAL	CA-C-O	-7.26	113.16	120.85
1	A	84	SER	N-CA-CB	7.16	120.75	110.16
2	D	60	VAL	N-CA-C	-7.15	103.56	110.42
1	A	81	SER	N-CA-C	7.13	119.67	111.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	THR	O-C-N	7.12	129.41	122.07
2	B	79	ASP	CA-CB-CG	7.12	119.72	112.60
2	B	46	GLY	CA-C-O	7.11	126.93	120.53
2	D	11	VAL	CB-CA-C	-7.09	102.90	111.97
2	B	54	VAL	N-CA-C	-7.07	103.89	110.53
2	D	43	GLU	CB-CA-C	-7.04	94.79	110.21
1	A	8	THR	CA-C-O	-7.04	113.43	120.82
2	D	28	LEU	N-CA-CB	7.02	120.55	110.16
1	C	118	THR	CA-CB-CG2	7.00	122.39	110.50
1	C	81	SER	N-CA-C	6.97	118.95	111.36
2	B	102	ASN	OD1-CG-ND2	-6.96	115.64	122.60
1	C	10	VAL	N-CA-CB	6.94	118.67	110.55
2	B	65	LYS	CA-CB-CG	-6.93	100.25	114.10
1	A	41	THR	CA-CB-OG1	6.92	119.98	109.60
1	A	92	ARG	NE-CZ-NH1	-6.87	114.64	121.50
2	D	135	ALA	CA-C-N	6.84	127.40	119.94
2	D	135	ALA	C-N-CA	6.84	127.40	119.94
2	D	92	HIS	N-CA-CB	6.78	120.78	110.28
1	C	14	TRP	CA-C-N	6.76	127.49	119.98
1	C	14	TRP	C-N-CA	6.76	127.49	119.98
2	D	139	ASN	CA-CB-CG	6.73	119.33	112.60
2	B	122	PHE	CA-C-N	6.70	131.58	120.86
2	B	122	PHE	C-N-CA	6.70	131.58	120.86
1	A	23	GLU	CA-C-O	-6.65	113.37	120.42
2	D	108	ASN	CA-C-O	-6.64	111.95	119.79
2	D	130	TYR	O-C-N	6.61	130.40	122.27
1	A	123	ALA	CB-CA-C	-6.60	100.25	110.81
1	A	85	ASP	CA-C-O	-6.60	113.91	120.70
2	D	113	VAL	CA-C-O	-6.56	113.89	120.85
2	B	101	GLU	N-CA-C	-6.56	104.17	111.71
1	A	131	SER	CA-C-O	-6.56	113.47	120.42
2	D	65	LYS	CA-C-O	6.55	127.51	119.97
1	A	43	PHE	O-C-N	-6.52	115.31	121.05
2	D	127	GLN	CA-C-O	6.45	127.39	120.55
2	D	54	VAL	CB-CA-C	-6.41	103.76	111.97
2	D	69	GLY	CA-C-N	-6.41	111.69	120.28
2	D	69	GLY	C-N-CA	-6.41	111.69	120.28
2	B	109	VAL	N-CA-C	-6.40	104.26	110.72
1	A	75	ASP	N-CA-CB	-6.38	104.13	111.79
2	B	69	GLY	N-CA-C	-6.38	104.61	112.77
1	C	64	ASP	CA-CB-CG	6.38	118.98	112.60
1	C	107	VAL	CA-C-O	-6.36	114.66	121.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ALA	N-CA-C	6.34	119.17	111.82
2	D	22	GLU	N-CA-C	6.32	118.25	111.36
2	B	45	PHE	CA-CB-CG	6.27	120.07	113.80
2	D	122	PHE	O-C-N	-6.27	114.87	122.71
2	D	21	ASP	CA-CB-CG	6.25	118.85	112.60
2	D	30	ARG	CD-NE-CZ	6.24	133.14	124.40
1	A	43	PHE	CA-C-O	6.24	127.06	121.07
1	A	132	VAL	CB-CA-C	-6.23	102.51	112.16
2	D	139	ASN	OD1-CG-ND2	-6.23	116.37	122.60
1	C	123	ALA	CB-CA-C	6.20	121.09	110.79
2	B	19	ASN	OD1-CG-ND2	-6.20	116.40	122.60
2	B	143	HIS	N-CA-C	6.20	118.84	111.71
1	C	92	ARG	NE-CZ-NH2	6.15	124.73	119.20
2	B	4	THR	CA-C-N	6.12	125.61	119.24
2	B	4	THR	C-N-CA	6.12	125.61	119.24
2	B	60	VAL	O-C-N	-6.08	115.95	121.91
1	C	61	LYS	CA-C-N	6.08	128.34	120.56
1	C	61	LYS	C-N-CA	6.08	128.34	120.56
2	D	11	VAL	N-CA-C	6.05	116.23	110.42
1	C	97	ASN	N-CA-C	6.03	118.81	111.82
1	C	130	ALA	O-C-N	6.03	129.02	122.15
1	A	101	LEU	CA-C-O	-6.02	114.03	120.42
2	B	42	PHE	O-C-N	-6.02	113.82	121.95
1	C	141	ARG	CD-NE-CZ	6.01	132.82	124.40
2	D	30	ARG	N-CA-CB	6.01	118.96	110.12
1	C	35	SER	CA-C-N	-6.00	115.78	123.16
1	C	35	SER	C-N-CA	-6.00	115.78	123.16
1	A	50	HIS	CA-CB-CG	-6.00	107.80	113.80
2	B	34	VAL	CA-C-O	-5.99	114.30	120.71
1	A	21	ALA	N-CA-C	5.99	118.30	111.11
1	A	33	PHE	CA-C-O	-5.99	113.34	120.10
2	D	126	VAL	O-C-N	5.99	128.00	121.83
2	B	40	ARG	CD-NE-CZ	5.95	132.73	124.40
1	C	127	LYS	CA-C-O	-5.93	114.26	120.55
2	B	42	PHE	N-CA-CB	-5.92	102.67	111.43
2	D	103	PHE	CA-C-O	5.92	126.69	120.42
1	C	53	ALA	N-CA-CB	5.92	119.45	110.28
2	B	94	ASP	N-CA-C	5.91	118.68	111.82
1	C	49	SER	N-CA-C	5.88	118.79	110.50
1	C	34	LEU	N-CA-CB	5.87	118.82	110.13
2	B	2	HIS	N-CA-C	5.87	117.76	108.67
2	B	9	SER	O-C-N	-5.84	115.39	122.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	N-CA-CB	5.83	118.69	110.12
1	C	10	VAL	CA-CB-CG1	5.83	120.31	110.40
1	C	73	VAL	CB-CA-C	-5.83	103.12	112.16
2	D	60	VAL	CA-C-O	-5.83	114.99	121.17
1	A	33	PHE	N-CA-C	5.82	118.41	111.71
2	D	22	GLU	N-CA-CB	5.82	118.77	110.16
1	A	131	SER	N-CA-CB	5.80	118.75	110.16
2	B	128	ALA	N-CA-C	5.77	117.56	111.28
2	B	96	LEU	N-CA-CB	-5.76	101.95	110.53
2	D	131	GLN	CB-CG-CD	5.75	122.38	112.60
1	C	140	TYR	CA-C-O	5.75	126.65	120.55
1	A	80	LEU	N-CA-CB	-5.75	102.13	110.70
2	D	49	SER	N-CA-C	5.75	120.35	113.23
1	C	73	VAL	N-CA-CB	5.74	120.47	110.65
2	B	117	HIS	CA-C-O	-5.73	114.81	120.82
2	B	107	GLY	O-C-N	-5.72	116.62	122.17
1	C	7	LYS	N-CA-C	-5.71	105.06	111.28
2	B	19	ASN	CB-CA-C	-5.71	101.41	111.05
2	D	87	THR	CA-C-O	-5.70	114.51	120.55
2	D	118	PHE	N-CA-C	5.70	120.50	113.50
1	A	29	LEU	CA-C-N	-5.69	112.66	120.28
1	A	29	LEU	C-N-CA	-5.69	112.66	120.28
1	C	39	THR	CA-CB-OG1	5.68	118.13	109.60
1	C	46	PHE	CA-CB-CG	5.68	119.48	113.80
1	A	36	PHE	N-CA-CB	-5.67	102.87	111.21
2	D	47	ASP	CA-C-O	5.67	127.37	120.62
2	D	2	HIS	N-CA-CB	-5.67	100.91	110.49
2	D	133	VAL	N-CA-C	5.64	115.83	110.42
2	D	138	ALA	CA-C-O	5.62	126.51	120.55
2	B	73	ASP	CA-C-N	5.62	126.22	119.98
2	B	73	ASP	C-N-CA	5.62	126.22	119.98
1	C	92	ARG	NH1-CZ-NH2	-5.61	112.00	119.30
1	A	24	TYR	N-CA-CB	5.61	118.46	110.16
1	C	37	PRO	N-CA-CB	5.61	109.58	103.30
1	C	113	LEU	CA-C-N	5.61	125.07	119.24
1	C	113	LEU	C-N-CA	5.61	125.07	119.24
1	A	80	LEU	CA-C-N	5.60	128.10	120.54
1	A	80	LEU	C-N-CA	5.60	128.10	120.54
2	D	135	ALA	CB-CA-C	5.60	121.42	110.67
1	A	126	ASP	CA-CB-CG	-5.59	107.01	112.60
2	B	73	ASP	CB-CG-OD1	5.57	131.22	118.40
1	A	68	ASN	CA-CB-CG	5.57	118.17	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	82	LYS	N-CA-C	5.57	117.81	111.02
2	B	87	THR	OG1-CB-CG2	-5.54	98.22	109.30
2	B	107	GLY	CA-C-O	5.53	126.22	120.80
1	C	83	LEU	CA-C-O	-5.53	114.56	120.42
2	D	45	PHE	CA-CB-CG	5.53	119.33	113.80
1	C	36	PHE	O-C-N	-5.52	116.40	121.37
2	D	30	ARG	NE-CZ-NH1	-5.51	115.98	121.50
1	C	79	ALA	CB-CA-C	-5.50	102.01	110.81
2	B	3	LEU	CA-CB-CG	-5.50	97.07	116.30
1	A	110	ALA	CB-CA-C	-5.49	100.48	110.63
1	C	118	THR	OG1-CB-CG2	5.48	120.27	109.30
2	B	4	THR	OG1-CB-CG2	5.48	120.26	109.30
1	C	89	HIS	N-CA-C	5.48	120.24	113.50
2	D	14	LEU	CA-C-O	-5.46	115.07	120.70
1	C	23	GLU	CB-CA-C	-5.46	102.30	110.88
1	A	113	LEU	CA-C-N	5.46	124.92	119.24
1	A	113	LEU	C-N-CA	5.46	124.92	119.24
1	C	114	PRO	O-C-N	-5.45	116.30	122.18
1	A	124	SER	CA-C-N	5.43	127.50	120.44
1	A	124	SER	C-N-CA	5.43	127.50	120.44
1	A	76	MET	CA-C-O	5.41	123.61	118.63
2	B	3	LEU	N-CA-C	-5.40	100.90	109.76
1	A	90	LYS	CB-CA-C	-5.40	104.05	112.31
1	C	85	ASP	CA-CB-CG	5.39	117.99	112.60
2	D	109	VAL	CA-C-O	5.39	126.30	120.47
1	A	76	MET	N-CA-C	5.38	120.25	113.25
1	A	45	HIS	CA-CB-CG	-5.37	108.43	113.80
1	A	132	VAL	O-C-N	-5.36	116.46	121.87
2	B	65	LYS	CB-CG-CD	-5.35	98.99	111.30
1	A	132	VAL	CA-C-N	5.35	127.88	120.29
1	A	132	VAL	C-N-CA	5.35	127.88	120.29
2	D	101	GLU	CB-CG-CD	5.34	121.69	112.60
2	B	88	LEU	O-C-N	5.34	128.84	122.27
2	D	26	GLU	CB-CG-CD	5.33	121.67	112.60
2	B	100	PRO	CA-C-O	5.33	126.93	118.89
1	A	78	ASN	CA-CB-CG	-5.32	107.28	112.60
2	B	98	VAL	N-CA-C	5.30	115.73	107.99
2	D	39	GLN	CB-CG-CD	-5.29	103.60	112.60
2	B	81	LEU	N-CA-CB	5.29	118.08	110.20
1	C	72	HIS	CA-C-O	-5.29	115.06	121.89
1	C	123	ALA	N-CA-CB	5.29	117.90	110.12
1	A	125	LEU	CA-C-N	5.29	127.31	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	LEU	C-N-CA	5.29	127.31	120.44
1	A	42	TYR	CA-C-O	-5.27	112.91	119.18
2	D	2	HIS	CB-CA-C	5.27	120.91	110.42
2	D	40	ARG	NE-CZ-NH1	-5.27	116.23	121.50
2	D	93	CYS	CA-C-O	5.27	126.42	120.89
1	A	26	ALA	CA-C-O	-5.26	114.97	120.55
2	B	30	ARG	CA-C-O	-5.26	113.93	119.97
1	C	85	ASP	CB-CA-C	-5.25	102.63	110.88
2	B	142	ALA	N-CA-CB	-5.25	102.42	110.44
2	D	82	LYS	CB-CA-C	-5.23	102.61	110.92
1	C	78	ASN	CB-CA-C	-5.23	101.96	110.85
1	A	10	VAL	N-CA-C	5.22	115.95	110.62
2	D	116	HIS	CB-CA-C	-5.21	102.71	110.88
2	B	18	VAL	CB-CA-C	-5.21	104.66	110.96
1	A	64	ASP	N-CA-CB	5.20	117.77	110.12
1	C	5	ALA	O-C-N	-5.19	116.62	122.12
1	A	58	HIS	CA-CB-CG	5.18	118.98	113.80
2	B	102	ASN	N-CA-CB	5.17	117.73	110.12
1	C	92	ARG	CD-NE-CZ	5.17	131.64	124.40
1	C	118	THR	CA-C-N	5.17	124.62	119.24
1	C	118	THR	C-N-CA	5.17	124.62	119.24
1	C	40	LYS	CA-C-O	5.17	125.74	119.38
1	C	46	PHE	N-CA-CB	5.17	118.62	110.56
1	A	66	LEU	CB-CA-C	5.17	119.06	110.90
2	D	60	VAL	O-C-N	5.16	126.97	121.91
1	A	20	HIS	N-CA-C	-5.16	106.83	113.02
1	C	90	LYS	CG-CD-CE	5.16	123.16	111.30
2	B	52	ASP	O-C-N	-5.15	116.66	122.12
2	B	124	PRO	O-C-N	-5.12	115.41	121.46
1	A	71	ALA	CA-C-O	-5.12	113.08	119.38
2	D	59	LYS	N-CA-CB	-5.12	102.41	110.30
1	C	100	LEU	N-CA-C	-5.12	105.61	111.14
2	D	94	ASP	N-CA-C	5.12	116.54	111.07
2	D	19	ASN	N-CA-C	-5.11	99.46	108.20
1	C	28	ALA	CA-C-O	-5.11	115.14	120.55
1	A	25	GLY	N-CA-C	-5.10	106.61	112.73
1	C	87	HIS	CA-C-O	-5.10	115.01	120.42
1	A	35	SER	CA-C-N	-5.10	116.89	123.16
1	A	35	SER	C-N-CA	-5.10	116.89	123.16
2	D	21	ASP	CA-C-O	-5.10	115.46	120.82
2	B	93	CYS	N-CA-CB	5.10	117.34	110.10
2	D	48	LEU	N-CA-C	-5.09	104.33	110.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	73	ASP	CB-CA-C	5.09	120.04	110.63
2	B	30	ARG	N-CA-CB	5.09	118.17	110.28
2	B	96	LEU	O-C-N	-5.07	115.78	122.42
2	B	143	HIS	CA-C-O	-5.07	114.37	120.10
2	B	6	GLU	N-CA-CB	5.06	118.02	110.22
1	C	30	GLU	CB-CA-C	5.06	119.97	110.70
2	B	54	VAL	CA-C-O	-5.06	115.43	121.05
2	B	67	VAL	CB-CA-C	-5.05	105.50	111.97
2	D	7	GLU	N-CA-C	-5.05	105.69	111.14
1	A	42	TYR	O-C-N	5.04	129.57	122.41
1	A	54	GLN	CA-CB-CG	5.04	124.18	114.10
2	B	112	CYS	CA-C-O	-5.04	115.21	120.55
1	C	127	LYS	CB-CA-C	-5.03	102.44	110.79
2	B	87	THR	CA-C-O	5.02	125.75	120.42
2	D	16	GLY	CA-C-O	-5.02	113.73	119.65
2	D	121	GLU	N-CA-C	-5.02	106.41	112.54
2	B	57	ASN	CB-CA-C	5.02	118.10	109.82
2	D	34	VAL	O-C-N	5.01	128.68	121.82
2	D	65	LYS	CA-C-N	5.01	127.25	120.44
2	D	65	LYS	C-N-CA	5.01	127.25	120.44
2	B	60	VAL	CA-C-O	5.00	126.47	121.17

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	134	VAL	CA
1	C	118	THR	CB
2	D	2	HIS	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	1	VAL	Peptide,Mainchain

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	1068	0	1073	22	0
1	C	1068	0	1073	20	0
2	B	1122	0	1117	33	0
2	D	1122	0	1118	23	0
3	A	43	0	30	2	0
3	B	43	0	30	2	0
3	C	43	0	30	0	0
3	D	43	0	30	2	0
4	B	5	0	0	0	0
5	A	74	0	0	2	0
5	B	88	0	0	5	0
5	C	57	0	0	1	0
5	D	47	0	0	0	0
All	All	4823	0	4501	95	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 11.

All (95) 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:107:GLY:HA3	2:B:134:VAL:HG21	1.31	1.10
2:D:4:THR:OG1	2:D:5:PRO:HD2	1.59	1.03
2:B:4:THR:HG21	5:B:438:HOH:O	1.56	1.01
2:B:107:GLY:CA	2:B:134:VAL:HG21	1.92	1.00
2:B:87:THR:HG22	5:B:468:HOH:O	1.62	0.99
2:D:8:LYS:NZ	2:D:79:ASP:OD2	2.01	0.93
2:B:80:ASN:O	2:B:84:THR:HG22	1.68	0.92
1:A:46:PHE:HA	1:A:54:GLN:HE22	1.34	0.92
2:B:144:LYS:CG	2:B:144:LYS:CE	2.52	0.86
2:B:4:THR:HG22	2:B:7:GLU:H	1.41	0.83
2:D:4:THR:OG1	2:D:5:PRO:CD	2.25	0.83
2:B:50:THR:HB	2:B:51:PRO:HD2	1.66	0.78
2:B:107:GLY:HA3	2:B:134:VAL:CG2	2.11	0.77
1:A:47:ASP:HB3	1:A:54:GLN:OE1	1.86	0.76
1:A:46:PHE:HA	1:A:54:GLN:NE2	2.01	0.74
2:B:80:ASN:O	2:B:84:THR:CG2	2.36	0.73
2:D:4:THR:HG23	2:D:7:GLU:H	1.56	0.71
2:B:2:HIS:N	2:B:2:HIS:CD2	2.62	0.67
1:A:47:ASP:CB	1:A:54:GLN:OE1	2.42	0.66
2:B:50:THR:HB	2:B:51:PRO:CD	2.26	0.66
2:B:29:GLY:O	2:B:33:VAL:HG23	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:PRO:HB2	2:B:125:PRO:HD3	1.80	0.63
1:A:141:ARG:HG3	1:C:127:LYS:HD2	1.81	0.63
1:C:118:THR:HG22	1:C:121:VAL:HB	1.81	0.62
2:D:4:THR:OG1	2:D:5:PRO:N	2.31	0.62
1:A:7:LYS:O	1:A:11:LYS:CG	2.48	0.60
2:B:4:THR:HG23	2:B:6:GLU:OE1	2.02	0.60
1:A:54:GLN:HG3	5:A:173:HOH:O	2.01	0.60
1:A:7:LYS:C	1:A:11:LYS:HE3	2.27	0.60
2:B:91:LEU:HD21	3:B:147:HEM:HBA1	1.82	0.59
2:B:24:GLY:N	2:B:68:LEU:HD12	2.17	0.59
1:C:7:LYS:NZ	1:C:74:ASP:OD1	2.31	0.59
2:D:19:ASN:CG	2:D:22:GLU:HG2	2.28	0.59
2:B:134:VAL:HG23	5:B:403:HOH:O	2.03	0.58
1:A:7:LYS:O	1:A:11:LYS:HE3	2.06	0.56
2:B:144:LYS:CG	2:B:144:LYS:HE2	2.35	0.56
2:D:4:THR:HG22	2:D:7:GLU:HG3	1.87	0.56
2:B:4:THR:HG22	2:B:7:GLU:N	2.18	0.55
2:D:110:LEU:HG	2:D:110:LEU:O	2.06	0.55
1:A:7:LYS:O	1:A:11:LYS:HG2	2.07	0.54
2:D:4:THR:HG23	2:D:7:GLU:N	2.21	0.54
1:A:31:ARG:O	1:A:35:SER:HB2	2.08	0.54
2:B:2:HIS:N	2:B:2:HIS:HD2	2.06	0.53
1:C:6:ASP:O	1:C:10:VAL:HG13	2.09	0.52
2:B:57:ASN:OD1	2:B:59:LYS:HB2	2.10	0.52
1:C:76:MET:N	1:C:77:PRO:CD	2.73	0.52
1:C:78:ASN:HB3	5:C:175:HOH:O	2.10	0.52
2:D:4:THR:O	2:D:5:PRO:C	2.52	0.52
1:A:47:ASP:H	1:A:54:GLN:CD	2.18	0.51
2:B:82:LYS:HE2	2:B:139:ASN:OD1	2.11	0.51
2:B:2:HIS:HB2	5:B:432:HOH:O	2.11	0.50
1:C:3:SER:O	1:C:6:ASP:HB2	2.12	0.50
2:D:68:LEU:HD22	2:D:71:PHE:HB3	1.95	0.49
1:A:31:ARG:HD3	2:B:127:GLN:OE1	2.13	0.48
2:B:77:HIS:HB2	2:B:84:THR:HG21	1.94	0.48
2:D:82:LYS:HA	2:D:140:ALA:HB1	1.95	0.48
1:A:7:LYS:O	1:A:11:LYS:HG3	2.15	0.47
1:C:43:PHE:N	1:C:44:PRO:CD	2.78	0.47
2:B:134:VAL:HG23	2:B:134:VAL:O	2.15	0.47
1:C:14:TRP:O	1:C:17:VAL:HB	2.15	0.46
1:C:118:THR:HG22	1:C:121:VAL:CB	2.43	0.46
2:B:91:LEU:CD2	3:B:147:HEM:HBA1	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:LYS:O	1:C:17:VAL:C	2.57	0.46
1:C:46:PHE:HB3	1:C:48:LEU:HD23	1.97	0.46
1:A:16:LYS:HG3	1:A:113:LEU:HD22	1.96	0.46
2:D:67:VAL:HG13	3:D:147:HEM:C3B	2.52	0.45
2:D:68:LEU:HD23	2:D:68:LEU:HA	1.80	0.45
1:C:6:ASP:OD2	1:C:127:LYS:HE2	2.17	0.44
1:C:118:THR:HG22	1:C:121:VAL:CG2	2.46	0.44
1:A:47:ASP:N	1:A:54:GLN:OE1	2.44	0.44
1:C:21:ALA:HB1	1:C:63:ALA:HB1	2.00	0.44
1:C:3:SER:H	1:C:6:ASP:HB2	1.82	0.43
1:A:93:VAL:HG11	3:A:142:HEM:CAC	2.48	0.43
1:A:7:LYS:HB3	1:A:11:LYS:HE3	2.00	0.43
1:A:118:THR:HB	1:A:119:PRO:HD2	2.01	0.43
2:B:123:THR:HA	5:B:407:HOH:O	2.19	0.43
2:D:82:LYS:HZ3	2:D:82:LYS:HG3	1.63	0.42
1:A:11:LYS:NZ	5:A:168:HOH:O	2.02	0.42
1:A:39:THR:HG22	1:A:97:ASN:HD22	1.83	0.42
2:D:30:ARG:HD2	2:D:113:VAL:HG22	2.01	0.42
1:C:123:ALA:HB2	2:D:34:VAL:HA	2.01	0.42
1:C:123:ALA:HB2	2:D:34:VAL:HG22	2.02	0.42
2:D:111:VAL:HG13	2:D:122:PHE:CZ	2.55	0.42
1:A:58:HIS:HE1	3:A:142:HEM:CHA	2.32	0.42
2:B:123:THR:HB	2:B:124:PRO:CD	2.50	0.42
2:B:111:VAL:HG11	2:B:131:GLN:OE1	2.19	0.41
2:D:11:VAL:HG13	2:D:130:TYR:CZ	2.55	0.41
2:B:38:THR:HG22	2:B:102:ASN:ND2	2.36	0.41
1:C:83:LEU:HD12	1:C:83:LEU:HA	1.95	0.41
2:D:85:PHE:O	2:D:86:ALA:C	2.62	0.41
3:D:147:HEM:CMC	3:D:147:HEM:HBC2	2.50	0.41
1:C:3:SER:N	1:C:6:ASP:HB2	2.36	0.41
2:D:82:LYS:HD3	2:D:143:HIS:CE1	2.57	0.40
2:B:81:LEU:HD23	2:B:81:LEU:HA	1.97	0.40
2:D:49:SER:C	2:D:50:THR:HG23	2.47	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%)	136 (98%)	3 (2%)	0	100	100
1	C	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
2	B	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	D	144/146 (99%)	140 (97%)	3 (2%)	1 (1%)	18	15
All	All	566/574 (99%)	552 (98%)	13 (2%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	2	HIS

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	113/113 (100%)	106 (94%)	7 (6%)	16	14
1	C	113/113 (100%)	104 (92%)	9 (8%)	11	8
2	B	118/118 (100%)	111 (94%)	7 (6%)	18	16
2	D	118/118 (100%)	108 (92%)	10 (8%)	10	7
All	All	462/462 (100%)	429 (93%)	33 (7%)	13	11

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	16	LYS
1	A	35	SER
1	A	52	SER
1	A	83	LEU
1	A	90	LYS
1	A	106	LEU
2	B	2	HIS
2	B	3	LEU
2	B	4	THR
2	B	59	LYS
2	B	75	LEU
2	B	84	THR
2	B	134	VAL
1	C	10	VAL
1	C	34	LEU
1	C	48	LEU
1	C	49	SER
1	C	60	LYS
1	C	73	VAL
1	C	90	LYS
1	C	113	LEU
1	C	118	THR
2	D	2	HIS
2	D	4	THR
2	D	65	LYS
2	D	68	LEU
2	D	73	ASP
2	D	78	LEU
2	D	82	LYS
2	D	84	THR
2	D	90	GLU
2	D	110	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	78	ASN
1	A	89	HIS
1	A	97	ASN
2	B	80	ASN
2	B	102	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	97	ASN
2	D	63	HIS
2	D	80	ASN
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](#)

5 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	147	2	50,50,50	1.55	11 (22%)	67,82,82	1.05	4 (5%)
3	HEM	C	142	1	50,50,50	1.46	9 (18%)	67,82,82	1.15	6 (8%)
3	HEM	A	142	1	50,50,50	1.64	10 (20%)	67,82,82	1.06	5 (7%)
4	SO4	B	402	-	4,4,4	1.86	1 (25%)	6,6,6	0.68	0
3	HEM	B	147	2	50,50,50	1.48	8 (16%)	67,82,82	2.61	24 (35%)

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	147	2	-	4/14/54/54	-
3	HEM	B	147	2	-	6/14/54/54	-
3	HEM	C	142	1	-	2/14/54/54	-
3	HEM	A	142	1	-	6/14/54/54	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	142	HEM	FE-NB	5.44	2.11	1.94
3	C	142	HEM	FE-NB	4.01	2.07	1.94
3	B	147	HEM	FE-ND	3.64	2.06	1.94
4	B	402	SO4	O1-S	3.51	1.65	1.44
3	D	147	HEM	FE-NB	3.50	2.05	1.94
3	B	147	HEM	CAB-C3B	3.39	1.56	1.47
3	A	142	HEM	FE-ND	3.32	2.05	1.94
3	C	142	HEM	FE-NC	3.31	2.06	1.95
3	D	147	HEM	FE-NC	3.24	2.05	1.95
3	C	142	HEM	FE-ND	3.23	2.04	1.94
3	D	147	HEM	CMC-C2C	3.05	1.57	1.50
3	D	147	HEM	FE-ND	2.94	2.04	1.94
3	B	147	HEM	O1A-CGA	2.84	1.31	1.22
3	D	147	HEM	CAC-C3C	2.79	1.54	1.47
3	A	142	HEM	CAD-C3D	2.78	1.58	1.51
3	A	142	HEM	CMC-C2C	2.77	1.56	1.50
3	D	147	HEM	CAB-C3B	2.63	1.54	1.47
3	A	142	HEM	FE-NC	2.62	2.03	1.95
3	A	142	HEM	CMB-C2B	2.58	1.56	1.50
3	D	147	HEM	CAA-C2A	2.56	1.57	1.51
3	B	147	HEM	CAD-C3D	2.56	1.57	1.51
3	A	142	HEM	CAB-C3B	2.53	1.54	1.47
3	B	147	HEM	FE-NB	2.52	2.02	1.94
3	B	147	HEM	FE-NA	2.44	2.03	1.95
3	C	142	HEM	CAB-C3B	2.41	1.53	1.47
3	D	147	HEM	CMA-C3A	2.37	1.55	1.50
3	A	142	HEM	CAC-C3C	2.34	1.53	1.47
3	C	142	HEM	C3D-C2D	-2.33	1.31	1.36
3	C	142	HEM	FE-NA	2.31	2.02	1.95
3	C	142	HEM	CMD-C2D	2.25	1.55	1.50
3	A	142	HEM	CMD-C2D	2.24	1.55	1.50
3	A	142	HEM	C2A-C3A	-2.23	1.33	1.38
3	B	147	HEM	CMB-C2B	2.20	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	142	HEM	CAC-C3C	2.15	1.53	1.47
3	B	147	HEM	CMA-C3A	2.14	1.55	1.50
3	D	147	HEM	CMD-C2D	2.12	1.55	1.50
3	D	147	HEM	C2A-C3A	-2.11	1.33	1.38
3	D	147	HEM	O1D-CGD	2.10	1.29	1.22
3	C	142	HEM	CMC-C2C	2.05	1.55	1.50

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	147	HEM	CAA-CBA-CGA	11.44	144.00	113.67
3	B	147	HEM	CBA-CAA-C2A	6.23	129.76	112.53
3	B	147	HEM	C3B-C2B-C1B	5.12	110.26	106.41
3	B	147	HEM	O2A-CGA-CBA	4.85	129.32	114.00
3	B	147	HEM	CHA-C4D-ND	4.73	130.22	124.37
3	B	147	HEM	O2A-CGA-O1A	-4.30	112.26	123.33
3	B	147	HEM	CAD-CBD-CGD	4.13	124.61	113.67
3	B	147	HEM	C1A-CHA-C4D	-4.03	116.76	126.25
3	B	147	HEM	CHB-C1B-NB	-4.00	119.42	124.37
3	C	142	HEM	CBA-CAA-C2A	3.82	123.09	112.53
3	B	147	HEM	C2B-C1B-NB	-3.77	105.50	109.84
3	C	142	HEM	CAA-CBA-CGA	3.73	123.57	113.67
3	B	147	HEM	CMB-C2B-C1B	-3.62	119.38	125.03
3	A	142	HEM	CBA-CAA-C2A	3.12	121.15	112.53
3	A	142	HEM	CHA-C1A-NA	2.88	129.09	123.86
3	B	147	HEM	C4A-C3A-C2A	2.81	110.04	106.82
3	D	147	HEM	CAD-CBD-CGD	2.79	121.06	113.67
3	C	142	HEM	CHC-C1C-NC	2.79	127.49	124.45
3	B	147	HEM	CHB-C1B-C2B	2.75	134.76	126.95
3	B	147	HEM	CAA-C2A-C3A	2.72	133.17	127.07
3	B	147	HEM	C4A-CHB-C1B	2.69	132.57	126.25
3	C	142	HEM	CHD-C1D-ND	2.69	127.32	124.42
3	B	147	HEM	O2D-CGD-CBD	2.69	122.49	114.00
3	C	142	HEM	C1C-CHC-C4B	-2.66	120.37	126.02
3	B	147	HEM	CHA-C4D-C3D	-2.62	120.40	125.23
3	D	147	HEM	O1D-CGD-CBD	-2.59	114.87	123.09
3	B	147	HEM	CHA-C1A-NA	2.55	128.48	123.86
3	A	142	HEM	C1A-CHA-C4D	-2.47	120.43	126.25
3	B	147	HEM	CHD-C1D-ND	-2.44	121.80	124.42
3	D	147	HEM	CHC-C1C-NC	2.38	127.04	124.45
3	B	147	HEM	O1D-CGD-CBD	-2.25	115.94	123.09
3	B	147	HEM	CMC-C2C-C1C	-2.25	120.76	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	142	HEM	CAD-CBD-CGD	2.22	119.55	113.67
3	D	147	HEM	C2A-C1A-NA	-2.19	107.72	110.15
3	B	147	HEM	CMA-C3A-C4A	-2.11	122.21	125.42
3	A	142	HEM	CAD-CBD-CGD	2.07	119.16	113.67
3	B	147	HEM	CHA-C1A-C2A	-2.06	120.79	125.30
3	B	147	HEM	CHD-C4C-NC	2.01	126.64	124.45
3	A	142	HEM	C2A-C1A-NA	-2.00	107.93	110.15

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	142	HEM	C2C-C3C-CAC-CBC
3	B	147	HEM	C2B-C3B-CAB-CBB
3	C	142	HEM	CAD-CBD-CGD-O2D
3	A	142	HEM	CAA-CBA-CGA-O1A
3	D	147	HEM	CAA-CBA-CGA-O2A
3	A	142	HEM	CAA-CBA-CGA-O2A
3	C	142	HEM	CAD-CBD-CGD-O1D
3	A	142	HEM	CAD-CBD-CGD-O1D
3	B	147	HEM	CAD-CBD-CGD-O1D
3	D	147	HEM	CAA-CBA-CGA-O1A
3	B	147	HEM	CAD-CBD-CGD-O2D
3	B	147	HEM	CAA-CBA-CGA-O1A
3	A	142	HEM	CAD-CBD-CGD-O2D
3	B	147	HEM	CAA-CBA-CGA-O2A
3	A	142	HEM	C4C-C3C-CAC-CBC
3	B	147	HEM	C4B-C3B-CAB-CBB
3	D	147	HEM	CAD-CBD-CGD-O2D
3	D	147	HEM	CAD-CBD-CGD-O1D

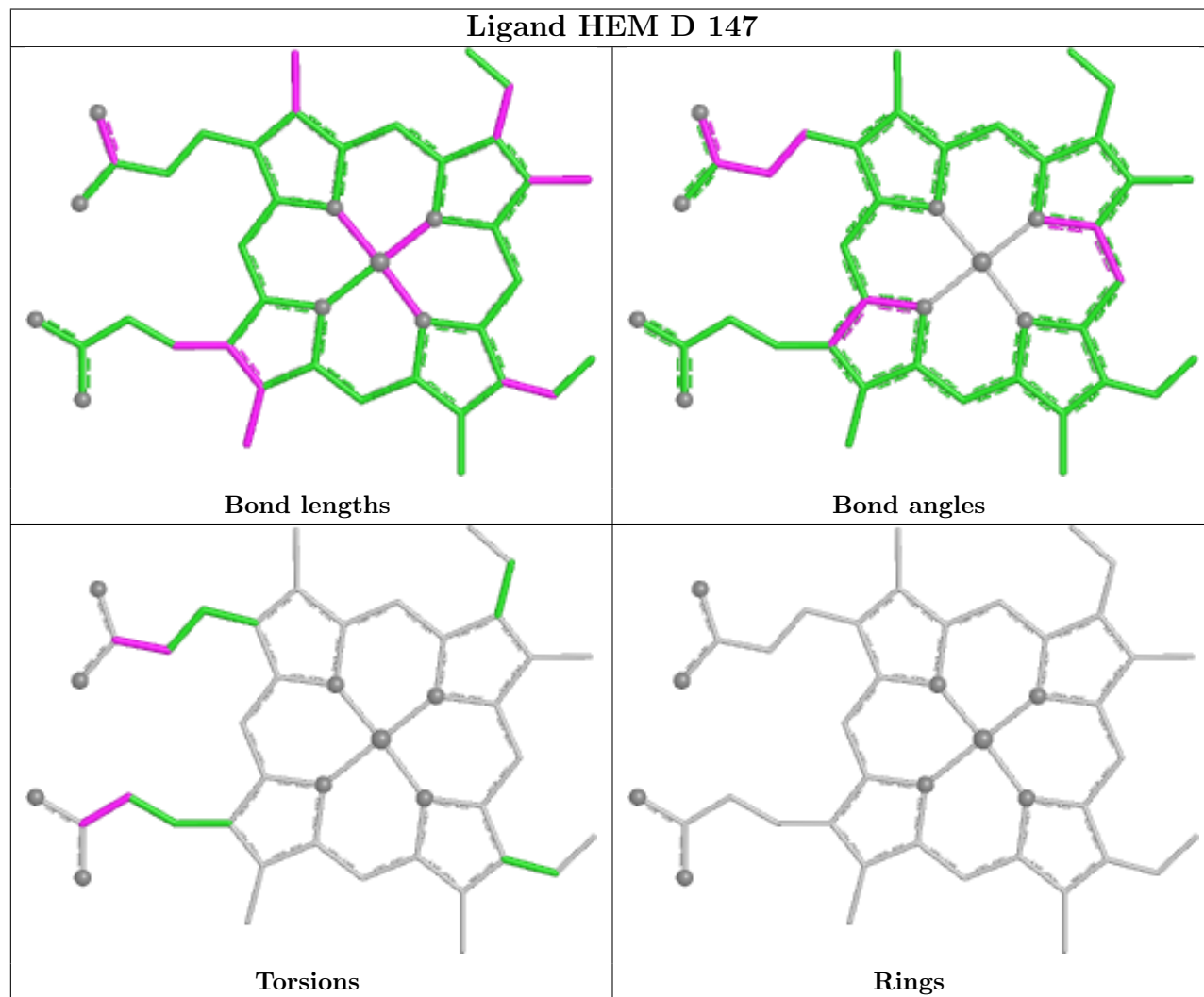
There are no ring outliers.

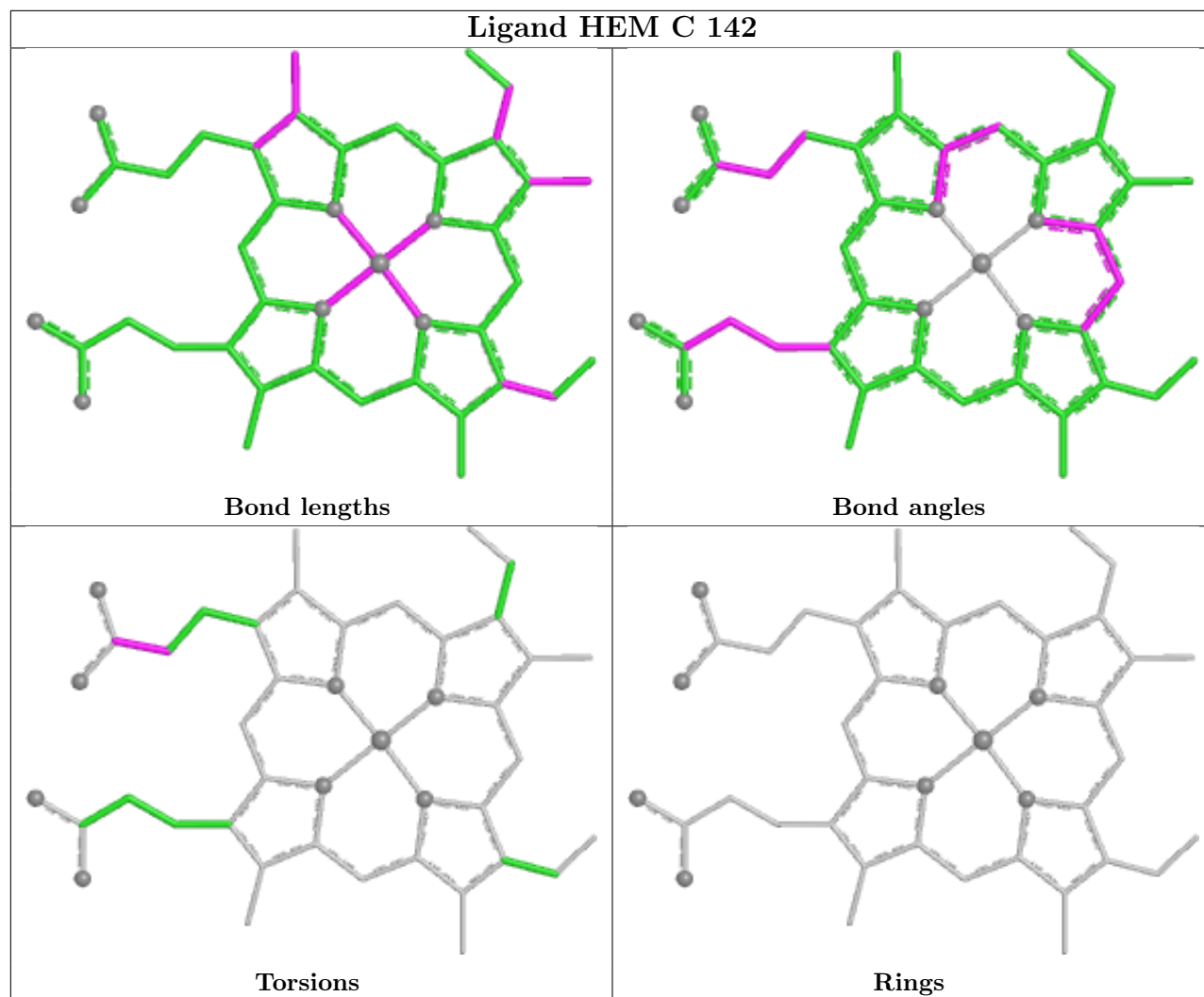
3 monomers are involved in 6 short contacts:

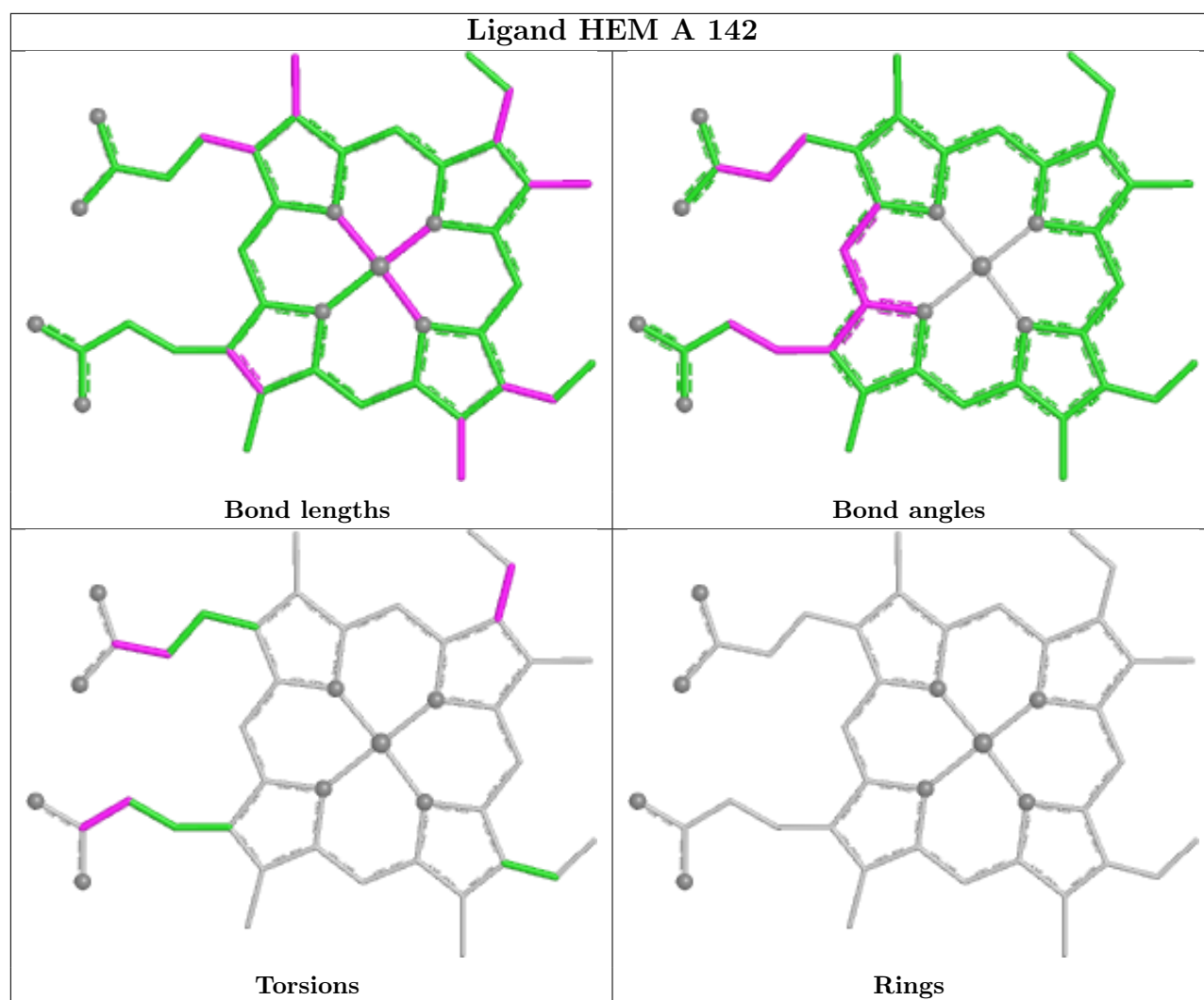
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	147	HEM	2	0
3	A	142	HEM	2	0
3	B	147	HEM	2	0

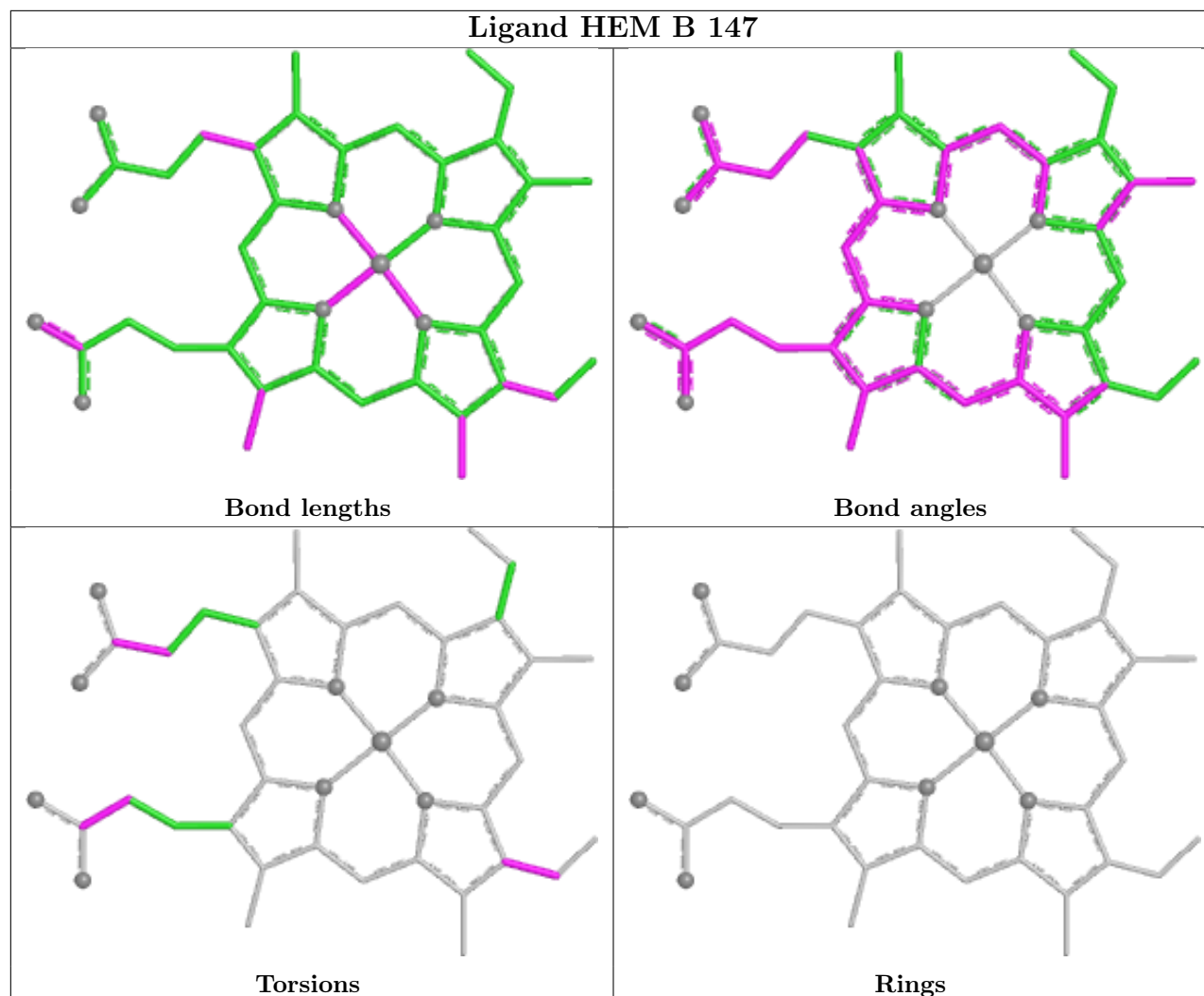
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1:VAL	C	2:HIS	N	1.82

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.