



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 10:42 AM EDT

PDB ID : 1NIH / pdb_00001nih
Title : Structure of deoxy-quaternary haemoglobin with liganded beta subunits
Authors : Luisi, B.; Liddington, B.
Deposited on : 1990-03-14
Resolution : 2.60 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

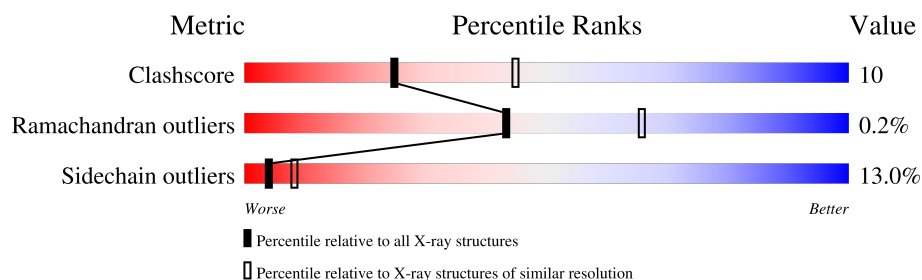
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HNI	A	201	X	-	-	-
3	HNI	C	201	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4648 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.

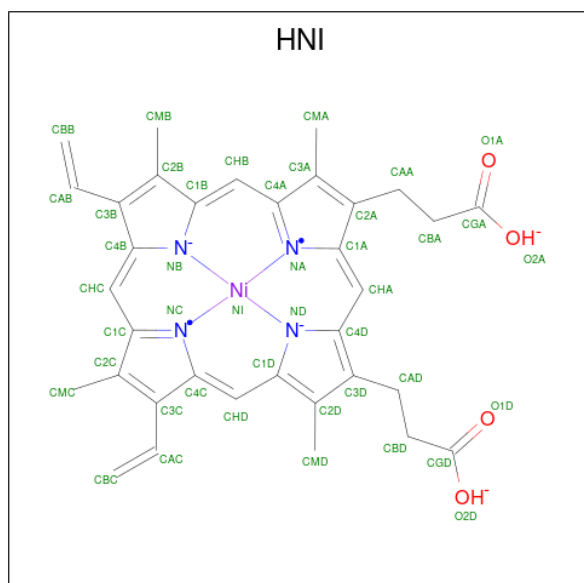
- Molecule 1 is a protein called HEMOGLOBIN (NICKELOUS DEOXY) (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	C	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			

- Molecule 2 is a protein called HEMOGLOBIN (FERROUS CARBONMONOXY) (BETA CHAIN).

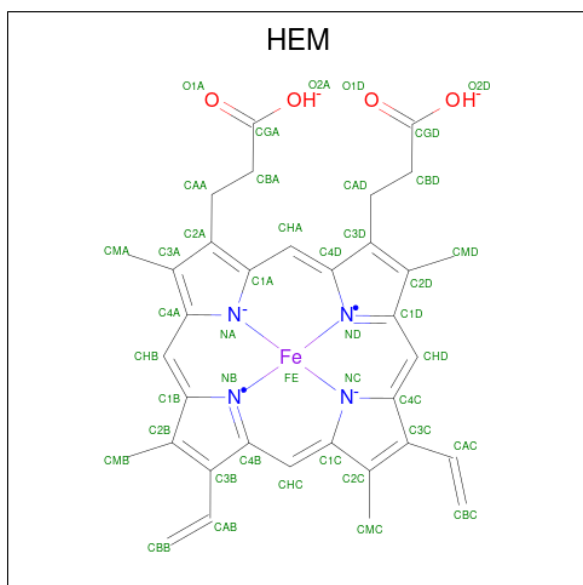
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	D	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			

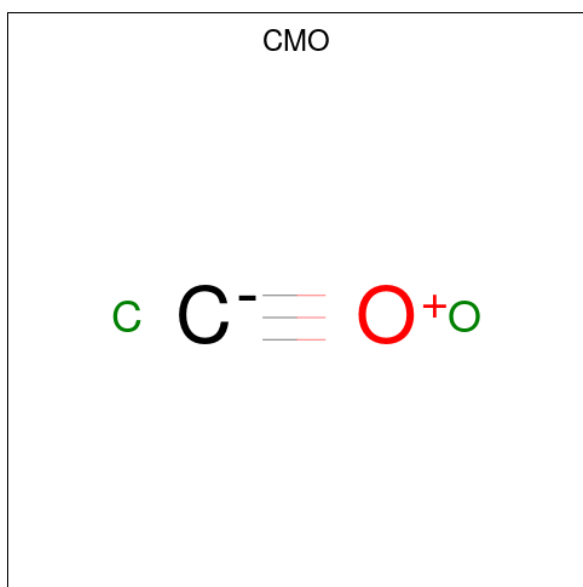
- Molecule 3 is PROTOPORPHYRIN IX CONTAINING NI(II) (CCD ID: HNI) (formula: $C_{34}H_{32}N_4NiO_4$).



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

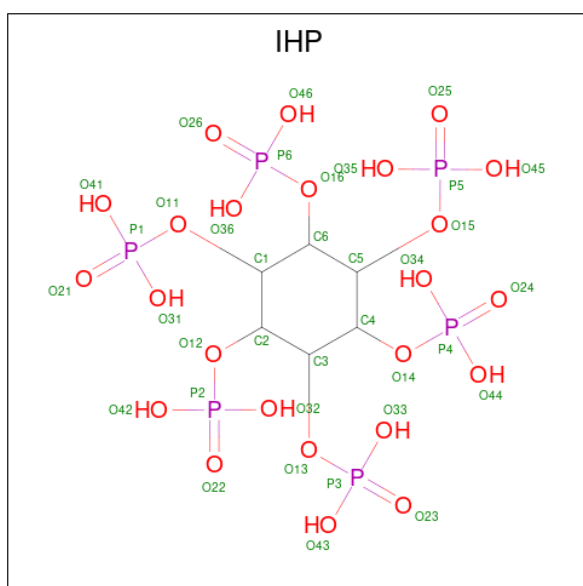
- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





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

- Molecule 6 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	P	0	0
			36	6	24	6		

- Molecule 7 is water.

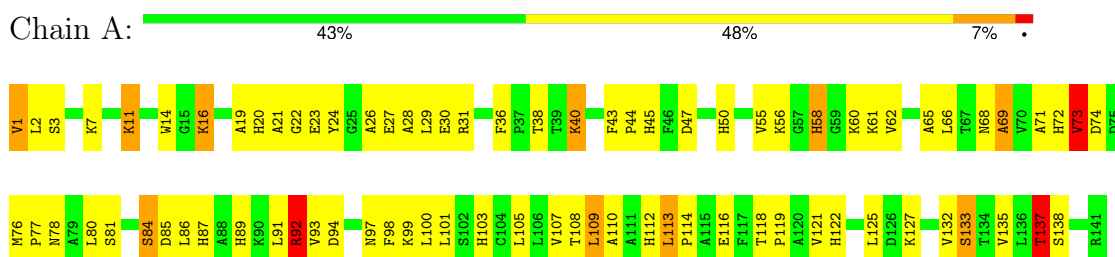
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	19	Total 19	O 19	0	0
7	B	13	Total 13	O 13	0	0
7	C	12	Total 12	O 12	0	0
7	D	8	Total 8	O 8	0	0

3 Residue-property plots

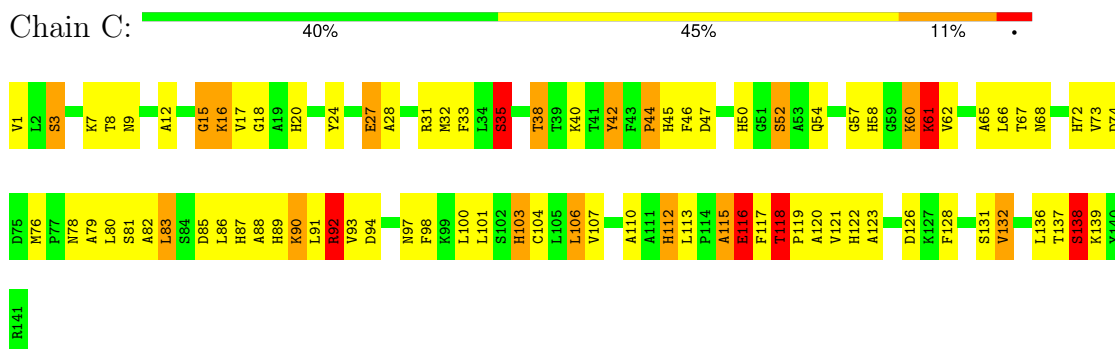
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

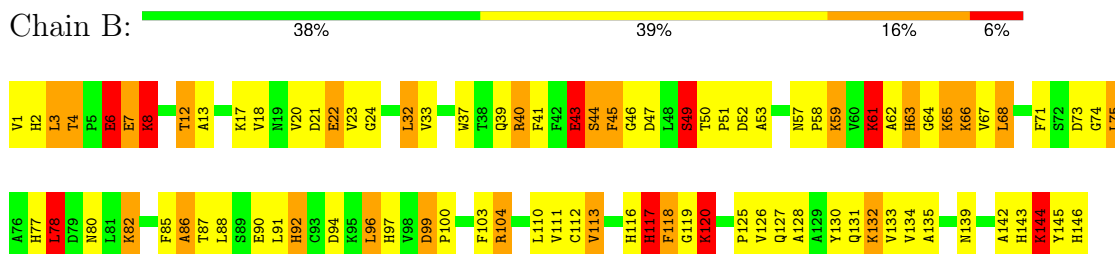
• Molecule 1: HEMOGLOBIN (NICKELOUS DEOXY) (ALPHA CHAIN)



• Molecule 1: HEMOGLOBIN (NICKELOUS DEOXY) (ALPHA CHAIN)



• Molecule 2: HEMOGLOBIN (FERROUS CARBONMONOXY) (BETA CHAIN)



• Molecule 2: HEMOGLOBIN (FERROUS CARBONMONOXY) (BETA CHAIN)





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	63.18Å 82.26Å 55.06Å 90.00° 98.42° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF	Depositor
R, R_{free}	0.214 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4648	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: CMO, HNI, IHP, 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	1.75	23/1097 (2.1%)	2.67	99/1491 (6.6%)
1	C	1.91	25/1097 (2.3%)	2.80	127/1491 (8.5%)
2	B	1.80	19/1153 (1.6%)	2.84	128/1566 (8.2%)
2	D	2.20	37/1153 (3.2%)	2.86	122/1566 (7.8%)
All	All	1.92	104/4500 (2.3%)	2.80	476/6114 (7.8%)

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
1	A	0	1
1	C	0	1
2	B	0	1
2	D	0	4
All	All	0	7

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	47	ASP	CG-OD2	30.10	1.82	1.25
1	C	50	HIS	ND1-CE1	12.60	1.45	1.32
2	D	97	HIS	ND1-CE1	11.27	1.43	1.32
1	A	20	HIS	ND1-CE1	10.93	1.43	1.32
1	A	89	HIS	ND1-CE1	10.47	1.43	1.32
1	C	89	HIS	ND1-CE1	10.45	1.43	1.32
2	B	117	HIS	CE1-NE2	10.24	1.42	1.32
2	D	143	HIS	CE1-NE2	10.21	1.42	1.32
2	B	143	HIS	ND1-CE1	10.19	1.42	1.32
1	C	20	HIS	CE1-NE2	10.07	1.42	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	HIS	CE1-NE2	9.96	1.42	1.32
2	B	2	HIS	ND1-CE1	9.89	1.42	1.32
1	A	20	HIS	CE1-NE2	9.86	1.42	1.32
1	C	72	HIS	ND1-CE1	9.74	1.42	1.32
2	B	2	HIS	CE1-NE2	9.63	1.42	1.32
2	D	2	HIS	ND1-CE1	9.53	1.42	1.32
1	C	50	HIS	CE1-NE2	9.15	1.41	1.32
2	D	116	HIS	CE1-NE2	9.14	1.41	1.32
1	C	89	HIS	CE1-NE2	9.09	1.41	1.32
2	B	143	HIS	CE1-NE2	9.08	1.41	1.32
2	B	92	HIS	CE1-NE2	8.95	1.41	1.32
1	C	122	HIS	ND1-CE1	8.87	1.41	1.32
1	A	89	HIS	CE1-NE2	8.81	1.41	1.32
2	D	97	HIS	CE1-NE2	8.79	1.41	1.32
2	D	146	HIS	ND1-CE1	8.70	1.41	1.32
2	B	146	HIS	ND1-CE1	8.54	1.41	1.32
2	D	3	LEU	N-CA	-8.35	1.35	1.46
2	B	97	HIS	CE1-NE2	8.26	1.40	1.32
2	B	97	HIS	ND1-CE1	8.23	1.40	1.32
2	D	2	HIS	C-N	-8.13	1.22	1.33
2	D	77	HIS	CE1-NE2	8.13	1.40	1.32
1	C	92	ARG	NE-CZ	8.03	1.41	1.33
2	B	77	HIS	ND1-CE1	7.92	1.40	1.32
2	D	49	SER	N-CA	7.83	1.56	1.46
1	A	45	HIS	ND1-CE1	7.77	1.40	1.32
1	C	72	HIS	CE1-NE2	7.77	1.40	1.32
1	C	122	HIS	CE1-NE2	7.65	1.40	1.32
2	D	146	HIS	CE1-NE2	7.61	1.40	1.32
2	B	77	HIS	CE1-NE2	7.60	1.40	1.32
2	D	116	HIS	ND1-CE1	7.57	1.40	1.32
2	B	50	THR	N-CA	7.52	1.54	1.45
2	D	117	HIS	ND1-CE1	7.21	1.39	1.32
2	D	67	VAL	CA-CB	-7.20	1.46	1.54
1	C	45	HIS	CE1-NE2	7.14	1.39	1.32
1	A	112	HIS	ND1-CE1	7.13	1.39	1.32
1	A	50	HIS	CE1-NE2	7.12	1.39	1.32
1	A	36	PHE	C-N	-7.07	1.26	1.34
2	D	99	ASP	C-N	-6.94	1.26	1.34
2	D	4	THR	C-N	-6.93	1.25	1.34
1	A	112	HIS	CE1-NE2	6.92	1.39	1.32
2	D	143	HIS	ND1-CE1	6.89	1.39	1.32
1	C	20	HIS	ND1-CE1	6.83	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	117	HIS	CE1-NE2	6.80	1.39	1.32
2	D	50	THR	N-CA	6.74	1.55	1.45
2	B	2	HIS	C-N	-6.73	1.23	1.33
1	A	72	HIS	CE1-NE2	6.66	1.39	1.32
2	B	92	HIS	ND1-CE1	6.58	1.39	1.32
1	A	112	HIS	CA-CB	-6.46	1.45	1.54
1	A	45	HIS	CD2-NE2	6.40	1.44	1.37
1	C	138	SER	N-CA	6.40	1.54	1.46
2	D	77	HIS	ND1-CE1	6.32	1.38	1.32
1	C	112	HIS	CG-CD2	6.29	1.42	1.35
1	C	112	HIS	ND1-CE1	6.21	1.38	1.32
2	D	64	GLY	C-N	-6.20	1.25	1.34
2	D	22	GLU	N-CA	6.18	1.54	1.46
1	A	138	SER	N-CA	6.18	1.54	1.46
1	A	122	HIS	CE1-NE2	6.16	1.38	1.32
2	D	53	ALA	N-CA	6.16	1.53	1.46
1	C	58	HIS	CE1-NE2	6.16	1.38	1.32
1	A	114	PRO	C-N	-6.13	1.25	1.33
2	D	92	HIS	CE1-NE2	6.08	1.38	1.32
1	A	103	HIS	ND1-CE1	6.07	1.38	1.32
1	A	72	HIS	ND1-CE1	6.03	1.38	1.32
1	A	87	HIS	CE1-NE2	5.99	1.38	1.32
2	B	7	GLU	C-N	-5.96	1.25	1.33
1	A	122	HIS	ND1-CE1	5.93	1.38	1.32
2	B	44	SER	C-N	5.91	1.42	1.33
2	D	108	ASN	C-N	5.90	1.41	1.33
1	A	50	HIS	ND1-CE1	5.76	1.38	1.32
2	D	2	HIS	CG-CD2	5.72	1.42	1.35
2	D	57	ASN	C-N	-5.71	1.26	1.34
2	D	146	HIS	CG-CD2	5.71	1.42	1.35
1	A	45	HIS	CE1-NE2	5.68	1.38	1.32
1	C	81	SER	C-N	-5.62	1.25	1.33
1	C	117	PHE	C-N	-5.57	1.23	1.33
2	D	100	PRO	N-CA	-5.57	1.40	1.47
2	D	39	GLN	C-N	-5.56	1.26	1.33
1	C	92	ARG	CD-NE	5.56	1.54	1.46
1	A	20	HIS	CG-CD2	5.44	1.41	1.35
1	C	119	PRO	C-N	-5.44	1.26	1.33
2	B	64	GLY	C-N	-5.40	1.26	1.33
2	D	77	HIS	C-N	-5.35	1.26	1.33
2	D	89	SER	CA-CB	-5.32	1.45	1.53
2	B	116	HIS	ND1-CE1	5.27	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	45	HIS	ND1-CE1	5.26	1.37	1.32
1	C	103	HIS	CE1-NE2	5.25	1.37	1.32
1	C	45	HIS	CD2-NE2	5.24	1.43	1.37
1	C	7	LYS	C-N	-5.21	1.26	1.33
1	A	36	PHE	CA-C	-5.20	1.46	1.52
2	D	22	GLU	C-N	5.19	1.39	1.33
2	B	117	HIS	ND1-CE1	5.18	1.37	1.32
2	D	143	HIS	N-CA	-5.12	1.40	1.46
2	D	2	HIS	CB-CG	5.10	1.57	1.50
1	C	87	HIS	CE1-NE2	5.08	1.37	1.32

All (476) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	139	ASN	CA-CB-CG	-22.41	90.19	112.60
2	D	143	HIS	CA-CB-CG	-16.16	97.64	113.80
2	D	79	ASP	CA-CB-CG	-13.95	98.65	112.60
2	D	2	HIS	CA-CB-CG	13.87	127.67	113.80
1	A	92	ARG	NE-CZ-NH2	-13.65	106.92	119.20
2	D	77	HIS	CA-CB-CG	-13.19	100.61	113.80
1	C	137	THR	CA-C-N	12.86	140.11	120.82
1	C	137	THR	C-N-CA	12.86	140.11	120.82
2	D	19	ASN	CA-C-O	-12.72	107.33	121.58
1	A	20	HIS	CA-CB-CG	12.39	126.19	113.80
1	C	16	LYS	CB-CG-CD	-12.36	82.88	111.30
1	C	87	HIS	CA-CB-CG	-11.95	101.85	113.80
1	C	85	ASP	CA-CB-CG	11.95	124.55	112.60
1	C	46	PHE	CA-CB-CG	11.10	124.90	113.80
2	D	47	ASP	OD1-CG-OD2	-10.89	96.76	122.90
1	A	132	VAL	CA-C-O	-10.78	109.73	120.95
2	D	43	GLU	CA-C-N	10.66	138.52	120.72
2	D	43	GLU	C-N-CA	10.66	138.52	120.72
2	B	94	ASP	CA-CB-CG	10.60	123.20	112.60
2	B	103	PHE	CA-C-O	-10.45	108.64	120.24
2	B	51	PRO	CA-C-N	-10.36	103.43	121.66
2	B	51	PRO	C-N-CA	-10.36	103.43	121.66
2	B	44	SER	CA-CB-OG	9.96	131.03	111.10
1	C	97	ASN	CA-CB-CG	-9.92	102.68	112.60
2	B	142	ALA	CA-C-N	9.81	133.82	120.38
2	B	142	ALA	C-N-CA	9.81	133.82	120.38
2	D	71	PHE	CA-CB-CG	-9.76	104.04	113.80
1	C	74	ASP	CA-CB-CG	9.74	122.34	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	97	HIS	CA-CB-CG	-9.65	104.15	113.80
2	B	61	LYS	O-C-N	9.55	132.02	122.09
2	D	2	HIS	CA-C-N	-9.53	109.11	122.93
2	D	2	HIS	C-N-CA	-9.53	109.11	122.93
1	C	18	GLY	CA-C-N	-9.51	105.16	122.38
1	C	18	GLY	C-N-CA	-9.51	105.16	122.38
2	B	90	GLU	O-C-N	-9.49	112.06	122.12
2	B	144	LYS	CG-CD-CE	9.47	133.08	111.30
2	B	117	HIS	CA-CB-CG	-9.44	104.36	113.80
2	B	116	HIS	CA-C-N	9.44	133.31	120.38
2	B	116	HIS	C-N-CA	9.44	133.31	120.38
1	A	137	THR	CA-C-N	9.30	139.29	121.54
1	A	137	THR	C-N-CA	9.30	139.29	121.54
2	B	104	ARG	CG-CD-NE	-9.28	91.59	112.00
1	A	58	HIS	ND1-CE1-NE2	9.24	117.64	108.40
2	B	52	ASP	CA-C-O	-9.14	108.58	119.27
2	D	105	LEU	CA-C-O	-9.12	111.25	120.82
1	C	120	ALA	CA-C-O	-9.05	111.38	120.70
1	C	92	ARG	CG-CD-NE	9.04	131.89	112.00
2	B	43	GLU	CB-CA-C	-9.03	93.93	110.63
2	D	3	LEU	CA-C-O	-9.02	111.15	120.71
1	C	78	ASN	CA-C-O	-8.98	111.45	120.70
2	B	21	ASP	CA-C-O	-8.89	111.66	121.00
2	B	117	HIS	ND1-CG-CD2	8.82	114.92	106.10
2	B	111	VAL	CA-C-O	-8.78	111.87	121.17
1	C	58	HIS	ND1-CE1-NE2	8.75	117.15	108.40
2	D	30	ARG	NE-CZ-NH2	-8.73	111.34	119.20
2	B	85	PHE	CA-C-O	-8.73	109.29	119.59
2	D	90	GLU	CB-CG-CD	-8.71	97.79	112.60
1	C	94	ASP	CA-CB-CG	-8.63	103.97	112.60
2	D	44	SER	CA-C-N	8.60	138.05	122.06
2	D	44	SER	C-N-CA	8.60	138.05	122.06
2	D	77	HIS	O-C-N	8.53	132.56	121.99
2	B	94	ASP	CA-C-N	-8.50	106.88	122.09
2	B	94	ASP	C-N-CA	-8.50	106.88	122.09
2	D	118	PHE	CA-CB-CG	-8.48	105.32	113.80
2	B	61	LYS	CA-C-N	8.43	131.40	120.44
2	B	61	LYS	C-N-CA	8.43	131.40	120.44
2	D	4	THR	O-C-N	-8.39	111.67	121.32
2	B	74	GLY	N-CA-C	-8.28	102.89	112.50
2	B	104	ARG	CA-C-O	-8.28	112.04	120.90
1	A	87	HIS	CA-CB-CG	-8.26	105.54	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	HIS	CA-CB-CG	-8.25	105.55	113.80
2	D	127	GLN	CA-C-O	-8.23	112.10	120.90
1	A	78	ASN	CA-C-O	-8.20	111.78	120.55
1	A	92	ARG	CD-NE-CZ	-8.17	112.96	124.40
2	B	40	ARG	NE-CZ-NH1	8.12	129.62	121.50
2	B	17	LYS	CA-C-O	-8.10	109.87	119.35
1	A	47	ASP	CA-C-O	-8.07	111.74	121.02
2	B	118	PHE	CA-CB-CG	-8.06	105.74	113.80
2	D	35	TYR	CA-C-N	8.05	127.77	119.56
2	D	35	TYR	C-N-CA	8.05	127.77	119.56
1	C	118	THR	CA-CB-OG1	8.00	121.60	109.60
2	B	117	HIS	N-CA-C	7.97	120.97	111.33
2	B	80	ASN	CA-CB-CG	7.95	120.55	112.60
2	B	52	ASP	CA-CB-CG	-7.91	104.69	112.60
1	C	118	THR	N-CA-CB	-7.90	98.88	109.78
1	C	3	SER	CA-C-N	7.89	128.31	119.32
1	C	3	SER	C-N-CA	7.89	128.31	119.32
1	C	47	ASP	CA-C-O	-7.86	111.37	120.49
1	C	17	VAL	O-C-N	7.84	129.59	121.91
2	D	62	ALA	CA-C-O	-7.74	112.69	120.82
1	A	77	PRO	CA-C-N	7.70	133.57	120.71
1	A	77	PRO	C-N-CA	7.70	133.57	120.71
2	D	21	ASP	O-C-N	-7.69	114.03	122.03
2	B	145	TYR	O-C-N	7.68	131.55	122.79
1	C	91	LEU	CA-C-O	-7.68	112.99	120.90
1	A	19	ALA	CA-C-N	7.64	134.41	122.26
1	A	19	ALA	C-N-CA	7.64	134.41	122.26
2	B	4	THR	CA-C-O	-7.62	112.49	120.87
1	C	16	LYS	CA-CB-CG	7.60	129.31	114.10
2	B	128	ALA	CA-C-N	7.58	130.76	120.44
2	B	128	ALA	C-N-CA	7.58	130.76	120.44
2	B	74	GLY	CA-C-O	-7.56	112.84	121.00
2	D	104	ARG	CA-CB-CG	7.55	129.20	114.10
2	B	96	LEU	CA-C-N	7.53	133.05	122.36
2	B	96	LEU	C-N-CA	7.53	133.05	122.36
1	C	35	SER	CA-C-O	7.47	128.34	119.60
1	C	118	THR	CA-C-O	-7.44	112.55	120.88
2	B	3	LEU	N-CA-C	-7.43	97.29	109.40
1	A	36	PHE	O-C-N	7.42	128.05	121.37
1	C	40	LYS	CD-CE-NZ	-7.40	88.22	111.90
2	B	104	ARG	CA-CB-CG	-7.39	99.32	114.10
2	B	128	ALA	CA-C-O	-7.39	111.75	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	HIS	CE1-NE2-CD2	-7.39	101.61	109.00
2	D	1	VAL	CB-CA-C	7.37	125.39	111.40
1	A	50	HIS	CA-C-O	7.34	128.96	120.96
2	B	73	ASP	CB-CA-C	-7.34	96.58	110.67
2	D	139	ASN	CB-CG-OD1	-7.33	106.14	120.80
2	B	80	ASN	CB-CG-ND2	-7.32	105.42	116.40
2	D	80	ASN	OD1-CG-ND2	7.30	129.90	122.60
1	A	28	ALA	O-C-N	7.29	129.68	122.09
1	C	97	ASN	CA-C-O	-7.29	111.59	119.97
1	C	101	LEU	CA-C-O	-7.29	113.17	120.82
2	D	116	HIS	O-C-N	7.24	129.53	122.07
1	C	118	THR	CA-C-N	7.24	127.57	119.32
1	C	118	THR	C-N-CA	7.24	127.57	119.32
2	D	127	GLN	O-C-N	7.24	129.62	122.09
1	C	61	LYS	CA-CB-CG	-7.23	99.64	114.10
1	A	135	VAL	CA-C-O	-7.21	113.21	120.85
2	B	22	GLU	CA-C-O	-7.20	112.79	120.42
2	D	6	GLU	CA-CB-CG	7.15	128.40	114.10
2	B	86	ALA	CA-C-N	-7.09	110.79	120.44
2	B	86	ALA	C-N-CA	-7.09	110.79	120.44
2	B	6	GLU	CA-C-O	-7.08	112.92	120.42
2	D	70	ALA	N-CA-C	7.07	119.84	111.71
2	D	109	VAL	CA-C-O	-7.07	113.60	120.95
2	D	20	VAL	CA-CB-CG2	7.06	122.41	110.40
2	B	88	LEU	CA-C-O	-7.06	110.95	119.49
1	A	122	HIS	CA-CB-CG	7.05	120.85	113.80
1	A	137	THR	CA-CB-CG2	7.04	122.47	110.50
2	D	47	ASP	CA-CB-CG	7.04	119.64	112.60
1	A	65	ALA	CA-C-O	-7.02	113.11	120.55
2	B	134	VAL	CA-C-O	-7.02	112.89	120.47
1	A	81	SER	CA-C-O	-7.01	113.12	120.55
2	B	74	GLY	O-C-N	6.98	128.88	122.18
2	D	113	VAL	CA-C-O	-6.97	113.78	121.17
1	C	115	ALA	N-CA-C	6.95	119.88	111.82
2	B	66	LYS	CA-C-O	-6.93	113.54	120.82
2	B	99	ASP	CA-CB-CG	6.93	119.53	112.60
1	A	78	ASN	CA-CB-CG	-6.92	105.68	112.60
1	C	31	ARG	NE-CZ-NH1	6.92	128.41	121.50
2	D	48	LEU	CA-C-N	6.91	132.40	120.58
2	D	48	LEU	C-N-CA	6.91	132.40	120.58
1	C	46	PHE	O-C-N	6.88	132.32	123.11
1	C	112	HIS	CA-CB-CG	6.84	120.64	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	43	GLU	CB-CG-CD	-6.84	100.98	112.60
1	C	80	LEU	CA-C-N	6.82	130.09	120.28
1	C	80	LEU	C-N-CA	6.82	130.09	120.28
1	A	127	LYS	CG-CD-CE	-6.81	95.63	111.30
1	C	54	GLN	CA-C-O	-6.79	112.70	120.24
1	C	98	PHE	CA-CB-CG	-6.77	107.03	113.80
1	A	86	LEU	N-CA-C	6.76	119.51	111.33
1	A	14	TRP	CA-CB-CG	-6.76	100.76	113.60
1	A	89	HIS	CA-CB-CG	6.73	120.53	113.80
2	B	17	LYS	CG-CD-CE	-6.72	95.84	111.30
1	C	79	ALA	CA-C-O	-6.71	112.68	120.20
2	D	35	TYR	O-C-N	6.71	127.53	121.42
1	A	11	LYS	CA-C-N	6.70	129.81	120.29
1	A	11	LYS	C-N-CA	6.70	129.81	120.29
2	B	3	LEU	CA-C-O	-6.67	113.50	120.70
2	D	21	ASP	CA-C-N	6.67	130.44	120.31
2	D	21	ASP	C-N-CA	6.67	130.44	120.31
2	B	20	VAL	O-C-N	6.66	130.63	121.84
2	D	87	THR	CA-C-O	-6.66	114.01	121.00
1	C	65	ALA	CA-C-O	-6.66	113.37	120.42
1	C	73	VAL	CA-C-N	-6.65	112.02	122.65
1	C	73	VAL	C-N-CA	-6.65	112.02	122.65
2	D	104	ARG	O-C-N	6.63	130.85	122.23
2	B	116	HIS	CA-CB-CG	-6.63	107.17	113.80
1	C	103	HIS	CA-C-O	-6.63	112.34	119.97
1	A	43	PHE	CA-CB-CG	-6.63	107.17	113.80
1	C	12	ALA	CA-C-N	6.61	129.43	120.44
1	C	12	ALA	C-N-CA	6.61	129.43	120.44
1	C	89	HIS	CA-CB-CG	-6.61	107.19	113.80
1	A	103	HIS	CA-C-O	-6.56	113.93	120.82
1	C	58	HIS	CE1-NE2-CD2	-6.56	102.44	109.00
1	C	20	HIS	ND1-CG-CD2	6.55	112.65	106.10
1	C	92	ARG	CB-CG-CD	-6.54	96.27	111.30
1	A	56	LYS	CA-C-O	-6.51	112.74	120.10
1	C	42	TYR	CA-CB-CG	-6.50	102.21	113.90
2	D	143	HIS	ND1-CG-CD2	6.49	112.59	106.10
1	A	133	SER	CA-CB-OG	-6.49	98.13	111.10
2	D	40	ARG	CA-C-O	-6.47	113.64	120.63
1	A	101	LEU	CA-C-O	-6.46	113.57	120.42
2	D	66	LYS	CA-CB-CG	6.46	127.02	114.10
2	B	40	ARG	CD-NE-CZ	6.46	133.44	124.40
2	B	110	LEU	CA-C-O	-6.46	113.57	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	ARG	CB-CG-CD	-6.45	96.46	111.30
2	B	97	HIS	CA-C-O	-6.43	114.38	121.84
1	A	23	GLU	CA-C-N	6.43	129.42	120.29
1	A	23	GLU	C-N-CA	6.43	129.42	120.29
2	D	11	VAL	CA-C-N	6.42	128.89	120.28
2	D	11	VAL	C-N-CA	6.42	128.89	120.28
1	A	100	LEU	CA-C-O	-6.39	113.14	120.24
2	D	87	THR	CB-CA-C	-6.37	101.15	110.96
2	D	85	PHE	CA-C-O	-6.37	111.74	119.32
1	C	100	LEU	CA-C-O	-6.37	114.14	120.70
1	A	113	LEU	CA-C-N	6.36	125.86	119.24
1	A	113	LEU	C-N-CA	6.36	125.86	119.24
1	A	27	GLU	CB-CG-CD	-6.35	101.80	112.60
2	D	50	THR	CA-CB-CG2	6.35	121.30	110.50
1	C	44	PRO	N-CD-CG	6.34	112.72	103.20
2	D	139	ASN	N-CA-C	6.33	118.70	111.11
1	C	40	LYS	CG-CD-CE	6.32	125.84	111.30
1	C	131	SER	CA-CB-OG	-6.31	98.48	111.10
1	A	68	ASN	CA-CB-CG	-6.29	106.31	112.60
1	A	94	ASP	CA-C-N	6.29	127.70	119.84
1	A	94	ASP	C-N-CA	6.29	127.70	119.84
1	A	36	PHE	CA-CB-CG	-6.29	107.51	113.80
2	D	57	ASN	CA-C-O	6.28	125.33	119.24
2	D	76	ALA	CA-C-N	6.27	133.94	122.54
2	D	76	ALA	C-N-CA	6.27	133.94	122.54
2	D	125	PRO	CA-C-O	-6.25	110.15	119.34
1	C	110	ALA	O-C-N	6.25	128.74	122.12
1	C	9	ASN	CA-CB-CG	-6.24	106.36	112.60
1	A	137	THR	N-CA-CB	-6.23	102.01	110.67
2	B	73	ASP	O-C-N	6.22	129.92	122.27
1	A	97	ASN	CA-C-N	6.22	128.61	120.28
1	A	97	ASN	C-N-CA	6.22	128.61	120.28
2	B	132	LYS	CA-CB-CG	6.21	126.52	114.10
1	A	21	ALA	O-C-N	6.21	128.54	122.09
1	C	82	ALA	N-CA-C	-6.21	105.86	113.50
1	C	91	LEU	CA-C-N	6.20	131.41	122.35
1	C	91	LEU	C-N-CA	6.20	131.41	122.35
1	C	67	THR	CA-C-O	-6.20	114.50	121.00
2	B	3	LEU	CB-CA-C	6.19	121.20	109.37
2	D	22	GLU	O-C-N	-6.19	114.66	122.27
1	A	85	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	72	HIS	CB-CA-C	-6.17	100.73	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	GLU	CA-CB-CG	-6.17	101.76	114.10
1	C	62	VAL	CA-C-O	-6.16	114.21	121.05
1	C	12	ALA	CA-C-O	-6.14	114.37	120.82
1	A	26	ALA	CA-C-O	-6.14	114.38	120.82
1	C	92	ARG	CA-C-N	6.13	130.38	121.18
1	C	92	ARG	C-N-CA	6.13	130.38	121.18
2	B	62	ALA	CA-C-N	-6.12	110.42	121.14
2	B	62	ALA	C-N-CA	-6.12	110.42	121.14
1	C	122	HIS	CA-CB-CG	6.12	119.92	113.80
1	C	138	SER	CA-C-O	6.12	127.77	120.92
2	D	57	ASN	CA-C-N	6.11	125.73	119.56
2	D	57	ASN	C-N-CA	6.11	125.73	119.56
2	D	134	VAL	CA-C-O	-6.11	113.87	120.47
2	B	104	ARG	CB-CA-C	-6.11	101.04	110.81
1	C	60	LYS	CA-C-O	-6.11	114.02	120.55
2	D	139	ASN	CB-CG-ND2	6.11	125.56	116.40
2	B	120	LYS	CB-CG-CD	6.10	125.33	111.30
2	D	143	HIS	CB-CG-CD2	-6.10	123.27	131.20
2	B	130	TYR	CA-C-O	-6.09	111.89	119.38
2	B	125	PRO	CA-N-CD	-6.07	103.50	112.00
2	B	13	ALA	CA-C-O	-6.07	112.99	119.97
2	D	50	THR	CA-C-N	6.07	126.23	119.32
2	D	50	THR	C-N-CA	6.07	126.23	119.32
2	D	133	VAL	CA-C-O	-6.07	114.64	120.95
2	D	137	VAL	CA-C-O	-6.06	114.75	121.17
1	C	52	SER	CA-C-O	-6.05	114.53	121.19
1	C	72	HIS	CA-C-O	-6.05	114.20	121.34
2	D	22	GLU	CA-C-O	-6.05	113.01	119.97
1	C	24	TYR	CA-C-O	-6.05	114.00	120.42
1	C	44	PRO	CA-N-CD	-6.05	103.53	112.00
2	D	121	GLU	CA-C-N	6.03	130.87	122.79
2	D	121	GLU	C-N-CA	6.03	130.87	122.79
1	A	40	LYS	CA-C-O	-6.03	112.20	119.49
2	B	71	PHE	N-CA-CB	-6.02	101.25	110.16
1	C	72	HIS	CA-C-N	6.02	130.64	120.64
1	C	72	HIS	C-N-CA	6.02	130.64	120.64
2	B	63	HIS	N-CA-CB	-6.02	100.59	110.40
1	C	87	HIS	N-CA-C	-6.02	104.64	111.14
1	C	16	LYS	CB-CA-C	-6.00	98.02	109.95
2	B	87	THR	CA-C-O	-5.99	114.53	120.70
1	C	115	ALA	CA-C-O	-5.99	113.08	119.97
2	D	142	ALA	O-C-N	5.99	131.17	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	8	THR	N-CA-CB	-5.98	101.40	110.07
2	D	24	GLY	O-C-N	5.97	130.47	122.70
2	B	133	VAL	CA-C-O	-5.96	114.44	121.05
1	A	73	VAL	N-CA-CB	-5.94	101.22	110.54
2	D	114	LEU	CA-C-O	-5.92	114.14	120.42
2	B	65	LYS	CA-C-O	-5.91	114.16	120.42
2	D	95	LYS	N-CA-C	-5.90	106.22	113.41
1	C	132	VAL	CA-C-N	5.89	128.18	120.28
1	C	132	VAL	C-N-CA	5.89	128.18	120.28
1	C	76	MET	CA-C-O	-5.89	112.09	120.16
2	D	121	GLU	CB-CG-CD	-5.88	102.61	112.60
1	C	50	HIS	CA-CB-CG	-5.88	107.92	113.80
2	B	52	ASP	O-C-N	5.88	130.51	122.46
2	B	104	ARG	O-C-N	5.87	128.20	122.09
2	D	77	HIS	ND1-CG-CD2	5.87	111.97	106.10
1	C	123	ALA	CA-C-O	-5.87	114.20	120.42
2	B	45	PHE	CA-CB-CG	-5.85	107.95	113.80
1	A	58	HIS	CA-CB-CG	-5.84	107.96	113.80
2	D	22	GLU	CA-CB-CG	5.83	125.77	114.10
1	C	119	PRO	O-C-N	5.82	128.93	122.24
1	C	93	VAL	CA-C-O	-5.80	113.93	120.95
2	D	77	HIS	CA-C-O	-5.80	115.16	121.20
1	A	76	MET	CA-C-O	-5.80	113.05	118.73
2	B	8	LYS	N-CA-CB	-5.79	101.38	110.30
2	B	66	LYS	CA-C-N	5.79	128.39	120.46
2	B	66	LYS	C-N-CA	5.79	128.39	120.46
2	D	53	ALA	CA-C-O	-5.78	114.72	120.90
2	D	133	VAL	CB-CA-C	-5.75	104.38	112.14
1	C	65	ALA	O-C-N	5.75	128.70	122.15
2	D	13	ALA	CA-C-N	5.75	128.29	120.54
2	D	13	ALA	C-N-CA	5.75	128.29	120.54
1	A	16	LYS	N-CA-CB	-5.74	101.67	110.16
1	A	71	ALA	CA-C-O	-5.73	114.34	120.42
2	B	61	LYS	CA-CB-CG	-5.73	102.64	114.10
1	C	112	HIS	CE1-NE2-CD2	-5.73	103.27	109.00
1	A	118	THR	CA-C-N	5.72	125.19	119.24
1	A	118	THR	C-N-CA	5.72	125.19	119.24
1	A	62	VAL	N-CA-C	-5.72	105.15	110.53
1	C	44	PRO	N-CA-CB	5.70	109.83	103.44
2	D	139	ASN	OD1-CG-ND2	5.70	128.30	122.60
2	D	40	ARG	NE-CZ-NH2	5.67	124.31	119.20
1	A	74	ASP	CA-CB-CG	-5.67	106.93	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	HIS	CA-C-O	-5.66	114.87	120.70
1	C	58	HIS	ND1-CG-CD2	5.66	111.76	106.10
1	C	112	HIS	ND1-CE1-NE2	5.66	114.06	108.40
1	A	22	GLY	CA-C-N	5.66	128.13	120.44
1	A	22	GLY	C-N-CA	5.66	128.13	120.44
2	B	85	PHE	CB-CA-C	-5.65	101.17	110.72
2	B	43	GLU	O-C-N	5.64	128.82	122.22
1	C	15	GLY	CA-C-O	-5.63	110.78	120.57
1	C	120	ALA	O-C-N	5.62	128.16	122.09
2	D	99	ASP	CA-CB-CG	5.61	118.21	112.60
1	C	126	ASP	CA-C-O	-5.61	114.48	120.42
1	A	87	HIS	O-C-N	5.60	128.14	122.09
2	D	12	THR	N-CA-CB	-5.59	101.90	110.12
1	C	31	ARG	CA-C-O	-5.59	114.63	120.55
2	B	78	LEU	N-CA-C	-5.58	106.43	113.18
2	B	139	ASN	CA-CB-CG	5.56	118.16	112.60
1	C	88	ALA	CA-C-O	-5.54	115.00	120.82
1	C	28	ALA	O-C-N	5.53	127.98	122.12
1	C	31	ARG	NE-CZ-NH2	-5.53	114.22	119.20
1	A	93	VAL	CA-C-O	-5.52	114.75	121.04
1	A	78	ASN	CA-C-N	-5.51	112.89	120.28
1	A	78	ASN	C-N-CA	-5.51	112.89	120.28
2	B	144	LYS	CA-CB-CG	-5.51	103.08	114.10
2	B	17	LYS	O-C-N	5.50	129.22	122.34
2	D	23	VAL	CA-CB-CG2	-5.50	101.05	110.40
1	A	58	HIS	CG-ND1-CE1	-5.50	99.95	109.30
2	B	139	ASN	CA-C-N	5.50	132.04	121.54
2	B	139	ASN	C-N-CA	5.50	132.04	121.54
2	B	145	TYR	CA-CB-CG	-5.50	104.01	113.90
2	D	117	HIS	ND1-CE1-NE2	5.50	113.90	108.40
1	A	92	ARG	NH1-CZ-NH2	5.49	126.44	119.30
2	D	139	ASN	N-CA-CB	-5.48	101.77	109.94
1	A	89	HIS	CA-C-O	-5.48	112.69	118.77
2	B	126	VAL	CA-C-O	-5.48	114.33	120.25
2	B	86	ALA	N-CA-C	-5.48	105.86	112.54
2	B	127	GLN	CA-C-O	-5.47	115.07	120.82
2	D	106	LEU	CA-C-N	5.47	126.01	119.94
2	D	106	LEU	C-N-CA	5.47	126.01	119.94
1	A	110	ALA	O-C-N	5.47	127.92	122.12
2	B	113	VAL	CA-C-O	-5.46	114.87	120.71
1	C	40	LYS	CB-CG-CD	-5.45	98.77	111.30
1	C	92	ARG	CA-CB-CG	5.45	125.00	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	43	GLU	N-CA-C	5.45	117.97	111.71
2	D	59	LYS	N-CA-C	-5.44	105.37	112.23
2	B	44	SER	N-CA-C	-5.44	106.48	113.01
1	A	58	HIS	ND1-CG-CD2	5.44	111.54	106.10
1	A	84	SER	CA-C-O	-5.44	113.72	119.97
2	B	53	ALA	O-C-N	5.44	127.67	122.07
2	D	68	LEU	CD1-CG-CD2	-5.43	98.85	110.80
1	A	94	ASP	CA-CB-CG	-5.42	107.18	112.60
2	B	77	HIS	CA-C-O	-5.41	111.73	122.23
2	B	99	ASP	CA-C-N	5.40	125.11	119.82
2	B	99	ASP	C-N-CA	5.40	125.11	119.82
1	A	1	VAL	CB-CA-C	5.40	121.66	111.40
1	C	86	LEU	CA-C-O	-5.40	113.76	119.97
2	B	131	GLN	CG-CD-NE2	5.39	124.49	116.40
2	B	100	PRO	CB-CA-C	-5.38	103.77	111.62
1	C	3	SER	O-C-N	-5.37	115.91	121.60
1	A	121	VAL	CA-C-O	-5.37	115.48	121.17
2	D	138	ALA	CA-C-N	5.37	127.78	120.54
2	D	138	ALA	C-N-CA	5.37	127.78	120.54
2	D	19	ASN	CB-CG-ND2	-5.37	108.35	116.40
2	D	53	ALA	O-C-N	5.37	127.67	122.09
2	D	108	ASN	CA-C-O	-5.37	114.28	120.24
1	C	33	PHE	CA-C-N	-5.36	111.66	121.52
1	C	33	PHE	C-N-CA	-5.36	111.66	121.52
1	A	87	HIS	N-CA-CB	5.36	117.83	110.07
2	B	37	TRP	CA-C-O	-5.35	113.01	119.49
2	D	40	ARG	N-CA-CB	-5.35	102.04	110.06
2	B	92	HIS	CA-CB-CG	5.34	119.14	113.80
2	B	131	GLN	O-C-N	5.34	128.84	122.27
1	C	66	LEU	CA-C-O	-5.33	114.77	120.42
1	C	12	ALA	O-C-N	5.33	127.56	122.07
1	C	104	CYS	CA-C-O	-5.33	114.77	120.42
1	A	31	ARG	CA-C-O	-5.33	114.90	120.55
1	C	58	HIS	CG-ND1-CE1	-5.32	100.26	109.30
2	B	135	ALA	CA-C-O	-5.31	114.92	120.55
1	A	107	VAL	CA-C-O	-5.30	115.24	120.85
2	D	80	ASN	CB-CG-ND2	-5.29	108.46	116.40
2	D	125	PRO	CA-N-CD	-5.29	104.59	112.00
1	C	32	MET	CA-C-O	-5.29	115.27	120.82
1	A	92	ARG	CG-CD-NE	5.29	123.63	112.00
2	D	6	GLU	CA-C-O	-5.28	114.28	120.20
2	B	49	SER	CA-C-O	-5.28	115.28	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ALA	CA-C-O	-5.28	114.95	120.55
1	A	55	VAL	CA-C-O	-5.28	115.58	121.17
1	C	128	PHE	CA-C-O	-5.28	114.83	120.42
2	D	1	VAL	CA-CB-CG2	5.26	119.34	110.40
2	D	95	LYS	CG-CD-CE	5.26	123.39	111.30
2	B	61	LYS	CB-CA-C	-5.26	102.40	110.81
2	B	112	CYS	CA-C-O	-5.25	114.98	120.55
1	A	61	LYS	CB-CA-C	-5.25	102.08	110.79
1	A	112	HIS	CA-C-N	5.24	129.44	123.21
1	A	112	HIS	C-N-CA	5.24	129.44	123.21
2	B	2	HIS	CA-C-N	-5.24	115.09	122.94
2	B	2	HIS	C-N-CA	-5.24	115.09	122.94
2	B	119	GLY	CA-C-N	5.24	128.98	120.60
2	B	119	GLY	C-N-CA	5.24	128.98	120.60
2	B	57	ASN	CA-C-O	5.23	124.67	119.75
2	D	117	HIS	CB-CG-CD2	-5.23	124.41	131.20
2	D	40	ARG	CB-CG-CD	-5.21	99.31	111.30
1	A	24	TYR	CA-C-O	-5.21	114.90	120.42
1	C	3	SER	CA-CB-OG	-5.21	100.69	111.10
1	C	92	ARG	CD-NE-CZ	-5.20	117.12	124.40
1	C	118	THR	OG1-CB-CG2	-5.20	98.90	109.30
1	A	89	HIS	O-C-N	-5.19	116.63	122.34
1	C	91	LEU	N-CA-C	-5.19	105.27	111.03
1	C	76	MET	CA-C-N	5.18	124.81	119.05
1	C	76	MET	C-N-CA	5.18	124.81	119.05
2	B	4	THR	N-CA-C	-5.17	102.75	110.20
1	C	9	ASN	CA-C-O	-5.17	115.39	120.82
1	C	103	HIS	CE1-NE2-CD2	-5.17	103.83	109.00
2	B	21	ASP	N-CA-C	-5.17	105.34	110.97
1	C	35	SER	CA-C-N	5.17	129.40	123.15
1	C	35	SER	C-N-CA	5.17	129.40	123.15
2	D	76	ALA	N-CA-C	5.17	119.57	113.16
2	B	132	LYS	CA-C-O	-5.17	114.94	120.42
1	A	108	THR	CA-C-O	-5.16	114.95	120.42
2	D	1	VAL	O-C-N	-5.16	114.75	123.00
1	C	116	GLU	CB-CG-CD	5.16	121.36	112.60
2	D	95	LYS	CB-CG-CD	5.16	123.16	111.30
2	D	126	VAL	CA-C-O	-5.15	115.39	120.85
1	C	47	ASP	CA-CB-CG	-5.15	107.45	112.60
1	A	92	ARG	NE-CZ-NH1	5.15	126.65	121.50
2	D	79	ASP	N-CA-C	-5.15	107.17	113.50
2	D	102	ASN	CA-CB-CG	-5.15	107.45	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ALA	CA-C-N	5.14	125.80	119.99
1	A	21	ALA	C-N-CA	5.14	125.80	119.99
2	B	144	LYS	CB-CG-CD	5.14	123.11	111.30
1	A	98	PHE	N-CA-C	-5.13	105.69	111.28
1	C	27	GLU	CA-C-O	-5.12	114.56	120.24
1	A	43	PHE	CA-C-O	-5.10	113.17	120.16
2	B	131	GLN	CG-CD-OE1	-5.08	110.64	120.80
2	B	33	VAL	CB-CA-C	-5.08	105.55	111.94
2	D	1	VAL	N-CA-CB	-5.06	102.89	111.50
2	B	21	ASP	CA-CB-CG	5.06	117.66	112.60
2	B	23	VAL	O-C-N	5.06	127.52	121.80
2	D	12	THR	CA-CB-CG2	5.05	119.09	110.50
2	D	59	LYS	CG-CD-CE	5.04	122.90	111.30
2	D	26	GLU	CB-CG-CD	-5.03	104.05	112.60
1	C	68	ASN	CA-CB-CG	-5.03	107.57	112.60
1	C	74	ASP	CA-C-O	-5.03	113.68	119.56
2	B	116	HIS	ND1-CG-CD2	5.02	111.12	106.10
2	D	78	LEU	CA-C-N	5.02	130.60	121.92
2	D	78	LEU	C-N-CA	5.02	130.60	121.92
1	C	20	HIS	CB-CA-C	-5.01	100.59	110.11
1	C	72	HIS	O-C-N	5.01	128.72	121.95
2	B	4	THR	CA-C-N	-5.01	114.50	119.56
2	B	4	THR	C-N-CA	-5.01	114.50	119.56
2	D	36	PRO	N-CD-CG	5.01	110.71	103.20
1	C	78	ASN	N-CA-CB	5.00	117.33	110.07
2	D	60	VAL	N-CA-C	-5.00	105.61	110.42
2	D	123	THR	O-C-N	5.00	126.90	121.60
1	A	119	PRO	O-C-N	5.00	127.58	122.18

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	92	ARG	Sidechain
2	B	104	ARG	Sidechain
1	C	92	ARG	Sidechain
2	D	104	ARG	Sidechain
2	D	30	ARG	Sidechain
2	D	40	ARG	Sidechain
2	D	47	ASP	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	1069	0	1073	16	0
1	C	1069	0	1073	19	6
2	B	1123	0	1118	26	30
2	D	1123	0	1118	36	35
3	A	43	0	30	0	0
3	C	43	0	30	0	0
4	B	43	0	30	3	0
4	D	43	0	30	0	1
5	B	2	0	0	0	0
5	D	2	0	0	0	0
6	B	36	0	6	5	0
7	A	19	0	0	1	0
7	B	13	0	0	4	0
7	C	12	0	0	1	1
7	D	8	0	0	1	5
All	All	4648	0	4508	89	43

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 (89) 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:47:ASP:OD2	2:D:47:ASP:CG	1.82	1.22
2:D:21:ASP:OD2	2:D:65:LYS:NZ	1.71	1.21
2:B:82:LYS:NZ	6:B:203:IHP:O43	1.73	1.20
2:D:21:ASP:CG	2:D:65:LYS:NZ	2.11	1.08
2:D:21:ASP:CG	2:D:65:LYS:HZ2	1.62	1.06
2:D:47:ASP:OD1	7:D:734:HOH:O	1.77	1.02
2:B:82:LYS:NZ	6:B:203:IHP:P3	2.35	0.99
2:D:91:LEU:HD12	2:D:95:LYS:HD3	1.53	0.91
2:B:86:ALA:HB1	2:B:144:LYS:HD2	1.55	0.89
2:B:24:GLY:HA2	2:B:68:LEU:HG	1.62	0.81
2:D:20:VAL:HG12	2:D:68:LEU:HB3	1.65	0.77
1:C:35:SER:OG	2:D:131:GLN:HG3	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:LYS:HZ1	6:B:203:IHP:P3	2.04	0.74
1:C:118:THR:HG22	1:C:121:VAL:H	1.55	0.72
2:B:4:THR:OG1	2:B:6:GLU:HG2	1.91	0.71
2:B:63:HIS:CE1	4:B:201:HEM:HBD2	2.27	0.69
2:D:21:ASP:CG	2:D:65:LYS:HZ3	1.89	0.69
2:B:82:LYS:HZ3	6:B:203:IHP:P3	2.00	0.67
1:A:40:LYS:NZ	2:D:146:HIS:OXT	2.22	0.67
2:B:86:ALA:HA	7:B:715:HOH:O	1.97	0.62
1:A:113:LEU:HB3	1:A:116:GLU:HB2	1.80	0.62
2:B:75:LEU:HA	2:B:78:LEU:HD11	1.82	0.61
2:D:21:ASP:HA	2:D:65:LYS:HD2	1.82	0.61
2:D:58:PRO:HA	2:D:61:LYS:HD2	1.83	0.60
1:A:92:ARG:HD3	2:D:40:ARG:HB2	1.84	0.60
2:B:40:ARG:HB3	1:C:92:ARG:HD3	1.84	0.60
2:D:22:GLU:OE2	2:D:117:HIS:HE1	1.85	0.59
1:A:44:PRO:HA	7:A:699:HOH:O	2.00	0.58
1:A:133:SER:O	1:A:137:THR:HB	2.04	0.57
1:C:103:HIS:HE1	2:D:131:GLN:OE1	1.87	0.56
2:B:47:ASP:OD1	2:B:49:SER:OG	2.25	0.55
2:D:91:LEU:CD1	2:D:95:LYS:HD3	2.31	0.53
2:B:63:HIS:O	2:B:67:VAL:HG23	2.08	0.53
2:D:135:ALA:O	2:D:139:ASN:HB2	2.08	0.53
1:C:38:THR:OG1	7:C:720:HOH:O	2.01	0.53
2:B:92:HIS:HA	2:B:96:LEU:HB2	1.91	0.52
2:D:24:GLY:N	2:D:68:LEU:HD12	2.25	0.52
1:A:92:ARG:HB3	2:D:37:TRP:HB2	1.92	0.52
2:D:5:PRO:HA	2:D:8:LYS:HB2	1.91	0.52
1:C:57:GLY:O	1:C:61:LYS:HG3	2.10	0.51
1:C:16:LYS:HD2	1:C:116:GLU:CD	2.36	0.51
2:D:3:LEU:HB2	2:D:8:LYS:HD2	1.93	0.50
2:B:86:ALA:HB2	7:B:715:HOH:O	2.10	0.50
1:C:27:GLU:OE1	1:C:112:HIS:HE1	1.94	0.50
2:B:86:ALA:CB	7:B:715:HOH:O	2.59	0.50
2:B:63:HIS:HE1	4:B:201:HEM:HBD2	1.75	0.49
2:D:50:THR:HB	2:D:51:PRO:HD2	1.94	0.49
1:C:35:SER:HG	2:D:131:GLN:HG3	1.78	0.48
2:D:31:LEU:HD22	2:D:106:LEU:HD13	1.96	0.47
2:D:51:PRO:O	2:D:55:MET:HG2	2.14	0.47
1:C:42:TYR:C	1:C:44:PRO:HD3	2.39	0.47
1:C:103:HIS:O	1:C:107:VAL:HG23	2.15	0.47
2:D:140:ALA:O	2:D:143:HIS:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:HIS:HE1	4:B:201:HEM:CHA	2.28	0.46
2:B:8:LYS:O	2:B:12:THR:HB	2.15	0.46
2:B:86:ALA:CA	7:B:715:HOH:O	2.58	0.46
2:D:42:PHE:O	2:D:45:PHE:HB2	2.15	0.46
1:C:116:GLU:H	1:C:116:GLU:HG2	1.20	0.46
2:D:143:HIS:ND1	2:D:144:LYS:HE2	2.31	0.46
2:B:113:VAL:O	2:B:117:HIS:HB2	2.17	0.45
1:C:138:SER:HB3	1:C:139:LYS:HG3	1.99	0.45
2:D:61:LYS:H	2:D:61:LYS:HG3	1.60	0.45
2:D:73:ASP:N	2:D:73:ASP:OD1	2.49	0.45
2:D:4:THR:O	2:D:7:GLU:HB2	2.17	0.45
2:D:14:LEU:HD22	2:D:14:LEU:HA	1.76	0.44
2:D:75:LEU:HA	2:D:78:LEU:HD13	2.00	0.43
1:C:113:LEU:HB3	1:C:116:GLU:HG3	2.00	0.43
2:B:43:GLU:H	2:B:43:GLU:HG2	1.69	0.43
1:A:7:LYS:HD3	1:A:73:VAL:HG13	2.01	0.42
1:A:7:LYS:O	1:A:11:LYS:HG3	2.19	0.42
1:A:69:ALA:HB2	1:A:80:LEU:HD21	2.01	0.42
1:A:91:LEU:HA	1:A:91:LEU:HD23	1.84	0.42
1:C:106:LEU:HD12	1:C:106:LEU:HA	1.76	0.42
1:C:132:VAL:O	1:C:136:LEU:HG	2.20	0.42
1:A:38:THR:HG21	2:D:100:PRO:HG2	2.00	0.41
1:A:66:LEU:HD23	1:A:66:LEU:HA	1.82	0.41
1:C:83:LEU:HD23	1:C:83:LEU:HA	1.67	0.41
2:D:3:LEU:HB3	2:D:7:GLU:CB	2.50	0.41
2:B:58:PRO:HA	2:B:61:LYS:HB2	2.01	0.41
1:A:2:LEU:HD23	1:A:2:LEU:HA	1.88	0.41
1:A:29:LEU:HD11	1:A:58:HIS:HD2	1.86	0.41
6:B:203:IHP:O22	6:B:203:IHP:H1	2.20	0.41
1:C:61:LYS:HB3	1:C:61:LYS:HE2	1.83	0.41
1:A:3:SER:O	1:A:7:LYS:HG3	2.21	0.41
2:B:7:GLU:OE2	2:B:132:LYS:HE3	2.21	0.40
2:B:32:LEU:HG	2:B:39:GLN:HG2	2.02	0.40
2:D:81:LEU:HA	2:D:81:LEU:HD23	1.77	0.40
2:B:99:ASP:OD2	1:C:42:TYR:OH	2.26	0.40
1:A:109:LEU:HD23	1:A:125:LEU:HD13	2.04	0.40

All (43) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:SER:O	2:D:95:LYS:CA[1_556]	0.79	1.41
2:B:44:SER:O	2:D:95:LYS:C[1_556]	0.82	1.38
2:B:41:PHE:CA	7:D:736:HOH:O[1_556]	1.08	1.12
2:B:41:PHE:C	7:D:736:HOH:O[1_556]	1.22	0.98
1:C:90:LYS:CE	2:D:59:LYS:CD[1_556]	1.30	0.90
2:D:5:PRO:CB	2:D:47:ASP:OD2[2_655]	1.32	0.88
1:C:90:LYS:NZ	2:D:59:LYS:CD[1_556]	1.36	0.84
2:B:44:SER:C	2:D:95:LYS:O[1_556]	1.45	0.75
2:B:44:SER:C	2:D:95:LYS:CA[1_556]	1.52	0.68
2:B:41:PHE:O	7:D:736:HOH:O[1_556]	1.54	0.66
2:B:59:LYS:CE	2:D:94:ASP:O[1_556]	1.60	0.60
2:B:44:SER:O	2:D:95:LYS:O[1_556]	1.64	0.56
2:D:9:SER:CB	2:D:49:SER:CB[2_655]	1.65	0.55
2:D:5:PRO:CG	2:D:47:ASP:OD2[2_655]	1.69	0.51
2:B:44:SER:CB	2:D:95:LYS:CB[1_556]	1.71	0.49
2:D:5:PRO:O	7:D:734:HOH:O[2_655]	1.75	0.45
2:B:44:SER:OG	2:D:95:LYS:CB[1_556]	1.80	0.40
2:D:5:PRO:CA	2:D:47:ASP:OD2[2_655]	1.84	0.36
2:B:43:GLU:OE2	4:D:201:HEM:O2D[1_556]	1.87	0.33
2:B:44:SER:O	2:D:95:LYS:N[1_556]	1.87	0.33
2:B:59:LYS:NZ	2:D:94:ASP:CB[1_556]	1.87	0.33
2:D:5:PRO:O	2:D:49:SER:OG[2_655]	1.88	0.32
2:B:44:SER:C	2:D:95:LYS:CB[1_556]	1.92	0.28
2:D:5:PRO:C	2:D:47:ASP:OD2[2_655]	1.92	0.28
2:B:118:PHE:O	7:C:730:HOH:O[1_455]	1.93	0.27
2:B:120:LYS:CB	1:C:115:ALA:CB[1_455]	1.94	0.26
2:B:44:SER:OG	2:D:95:LYS:CG[1_556]	2.01	0.19
2:B:45:PHE:N	2:D:95:LYS:O[1_556]	2.02	0.18
2:B:120:LYS:CB	1:C:116:GLU:OE2[1_455]	2.03	0.17
2:D:6:GLU:OE1	2:D:47:ASP:CG[2_655]	2.03	0.17
2:B:59:LYS:CE	2:D:94:ASP:C[1_556]	2.04	0.16
2:B:44:SER:CA	2:D:95:LYS:C[1_556]	2.05	0.15
2:B:46:GLY:CA	2:D:97:HIS:NE2[1_556]	2.05	0.15
2:B:44:SER:OG	2:D:95:LYS:CD[1_556]	2.06	0.14
2:B:44:SER:O	2:D:96:LEU:N[1_556]	2.06	0.14
2:B:59:LYS:NZ	2:D:94:ASP:CA[1_556]	2.07	0.13
2:B:44:SER:O	2:D:95:LYS:CB[1_556]	2.09	0.11
1:C:90:LYS:CE	2:D:59:LYS:CE[1_556]	2.09	0.11
1:C:90:LYS:CD	2:D:59:LYS:CE[1_556]	2.11	0.09
2:B:41:PHE:CB	7:D:736:HOH:O[1_556]	2.13	0.07
2:B:44:SER:CA	2:D:95:LYS:CB[1_556]	2.13	0.07
2:D:6:GLU:N	2:D:47:ASP:OD1[2_655]	2.16	0.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:LYS:CD	2:D:94:ASP:O[1_556]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
1	C	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	18	38
2	B	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	D	144/146 (99%)	137 (95%)	7 (5%)	0	100	100
All	All	566/574 (99%)	538 (95%)	27 (5%)	1 (0%)	43	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	15	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/113 (100%)	104 (92%)	9 (8%)	11	25
1	C	113/113 (100%)	100 (88%)	13 (12%)	5	11
2	B	118/118 (100%)	96 (81%)	22 (19%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	118/118 (100%)	102 (86%)	16 (14%)	3	7
All	All	462/462 (100%)	402 (87%)	60 (13%)	4	8

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	16	LYS
1	A	60	LYS
1	A	73	VAL
1	A	84	SER
1	A	99	LYS
1	A	105	LEU
1	A	109	LEU
1	A	137	THR
2	B	1	VAL
2	B	3	LEU
2	B	6	GLU
2	B	8	LYS
2	B	12	THR
2	B	18	VAL
2	B	22	GLU
2	B	32	LEU
2	B	43	GLU
2	B	49	SER
2	B	59	LYS
2	B	61	LYS
2	B	65	LYS
2	B	66	LYS
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	82	LYS
2	B	91	LEU
2	B	117	HIS
2	B	120	LYS
2	B	144	LYS
1	C	1	VAL
1	C	3	SER
1	C	35	SER
1	C	38	THR
1	C	52	SER

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Mol	Chain	Res	Type
1	C	60	LYS
1	C	61	LYS
1	C	83	LEU
1	C	90	LYS
1	C	106	LEU
1	C	116	GLU
1	C	118	THR
1	C	138	SER
2	D	2	HIS
2	D	6	GLU
2	D	8	LYS
2	D	12	THR
2	D	14	LEU
2	D	20	VAL
2	D	26	GLU
2	D	32	LEU
2	D	40	ARG
2	D	43	GLU
2	D	44	SER
2	D	49	SER
2	D	68	LEU
2	D	75	LEU
2	D	78	LEU
2	D	95	LYS

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	103	HIS
2	B	63	HIS
2	B	108	ASN
2	B	143	HIS
1	C	103	HIS
1	C	112	HIS
2	D	2	HIS
2	D	80	ASN
2	D	117	HIS

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 ⓘ

7 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$
4	HEM	B	201	2	50,50,50	1.42	7 (14%)	67,82,82	1.76	22 (32%)
3	HNI	A	201	-	50,50,50	1.09	5 (10%)	67,82,82	1.53	12 (17%)
4	HEM	D	201	2	50,50,50	2.05	4 (8%)	67,82,82	1.52	12 (17%)
5	CMO	B	202	-	0,1,1	-	-	-	-	-
3	HNI	C	201	-	50,50,50	1.26	7 (14%)	67,82,82	1.46	14 (20%)
5	CMO	D	202	-	0,1,1	-	-	-	-	-
6	IHP	B	203	-	36,36,36	1.28	6 (16%)	60,60,60	1.14	4 (6%)

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
4	HEM	B	201	2	-	5/14/54/54	-
3	HNI	A	201	-	1/1/3/9	4/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	D	201	2	-	3/14/54/54	-
3	HNI	C	201	-	1/1/3/9	2/14/54/54	-
6	IHP	B	203	-	-	6/30/54/54	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	201	HEM	FE-NB	10.16	2.26	1.94
4	D	201	HEM	FE-ND	-7.36	1.72	1.94
4	B	201	HEM	FE-NB	5.40	2.11	1.94
3	C	201	HNI	NI-NC	3.30	2.03	1.93
6	B	203	IHP	P4-O14	3.18	1.65	1.59
4	B	201	HEM	FE-NC	-3.08	1.85	1.95
3	C	201	HNI	NI-ND	-3.03	1.83	1.93
3	C	201	HNI	NI-NA	-2.96	1.83	1.93
6	B	203	IHP	C6-C1	2.79	1.58	1.52
3	A	201	HNI	NI-NA	-2.57	1.85	1.93
4	B	201	HEM	C3C-C4C	-2.57	1.41	1.46
6	B	203	IHP	P2-O12	2.46	1.63	1.59
3	C	201	HNI	CBB-CAB	2.44	1.42	1.30
4	D	201	HEM	O2D-CGD	-2.44	1.22	1.30
3	A	201	HNI	O2D-CGD	-2.43	1.22	1.30
3	C	201	HNI	O2A-CGA	-2.40	1.22	1.30
3	C	201	HNI	O2D-CGD	-2.39	1.22	1.30
4	D	201	HEM	CBC-CAC	2.33	1.41	1.30
6	B	203	IHP	P3-O13	2.23	1.63	1.59
4	B	201	HEM	C1D-ND	2.20	1.43	1.38
4	B	201	HEM	C4A-NA	2.15	1.43	1.39
3	A	201	HNI	O2A-CGA	-2.14	1.23	1.30
3	C	201	HNI	C1D-ND	2.14	1.42	1.38
6	B	203	IHP	P5-O15	2.08	1.63	1.59
3	A	201	HNI	C3D-C2D	-2.07	1.33	1.38
4	B	201	HEM	CHC-C1C	2.05	1.42	1.38
3	A	201	HNI	NI-NC	2.04	1.99	1.93
6	B	203	IHP	C6-C5	2.02	1.56	1.52
4	B	201	HEM	CBB-CAB	2.01	1.40	1.30

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	201	HEM	CAD-CBD-CGD	-4.65	101.33	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	201	HEM	C4C-CHD-C1D	-4.25	116.98	126.02
4	B	201	HEM	CHC-C1C-NC	4.18	129.00	124.45
4	D	201	HEM	C4D-ND-C1D	-3.84	100.66	105.21
3	A	201	HNI	CAB-C3B-C4B	-3.56	116.31	124.82
3	A	201	HNI	CHC-C4B-C3B	-3.47	119.36	125.21
3	C	201	HNI	C4B-C3B-C2B	-3.38	103.89	106.81
4	B	201	HEM	C2A-C1A-NA	3.31	113.82	110.15
3	C	201	HNI	CMC-C2C-C1C	-3.24	119.97	125.03
4	B	201	HEM	CAA-C2A-C1A	-2.95	119.17	124.94
3	A	201	HNI	C1B-CHB-C4A	-2.91	119.84	126.02
4	B	201	HEM	C4D-ND-C1D	-2.90	101.78	105.21
6	B	203	IHP	C5-C4-C3	2.87	116.73	110.43
3	C	201	HNI	CAA-CBA-CGA	-2.85	106.10	113.67
4	D	201	HEM	CMC-C2C-C1C	-2.85	119.71	124.73
4	D	201	HEM	CBA-CAA-C2A	2.83	120.35	112.53
3	A	201	HNI	C2A-C1A-NA	2.78	113.95	111.02
3	A	201	HNI	CAB-C3B-C2B	2.76	137.42	128.43
4	B	201	HEM	CMA-C3A-C4A	-2.76	121.21	125.42
4	D	201	HEM	C2D-C1D-ND	2.72	113.05	109.90
4	B	201	HEM	O1A-CGA-CBA	-2.71	114.51	123.09
4	D	201	HEM	O2A-CGA-CBA	2.66	122.40	114.00
3	C	201	HNI	C4D-ND-C1D	-2.64	100.28	105.28
4	B	201	HEM	CAA-C2A-C3A	2.62	132.95	127.07
4	D	201	HEM	O1A-CGA-CBA	-2.61	114.81	123.09
4	B	201	HEM	CBD-CAD-C3D	2.61	119.75	112.53
3	A	201	HNI	CHC-C4B-NB	2.58	127.65	124.64
3	A	201	HNI	CBA-CAA-C2A	2.56	119.61	112.53
4	B	201	HEM	C3C-C2C-C1C	2.56	109.47	107.05
4	B	201	HEM	O1D-CGD-CBD	-2.52	115.09	123.09
4	B	201	HEM	O2D-CGD-CBD	2.50	121.89	114.00
4	D	201	HEM	C3B-C4B-NB	2.49	111.26	109.47
6	B	203	IHP	P2-O12-C2	-2.46	116.87	123.43
3	C	201	HNI	C4D-CHA-C1A	-2.39	120.62	126.25
3	A	201	HNI	CHA-C1A-C2A	-2.34	120.92	125.23
3	A	201	HNI	CMC-C2C-C1C	-2.33	121.39	125.03
3	A	201	HNI	C1A-NA-C4A	-2.31	100.89	105.25
3	C	201	HNI	CHB-C4A-C3A	-2.25	121.47	125.03
3	C	201	HNI	C2A-C1A-NA	2.22	113.36	111.02
4	B	201	HEM	C3B-C4B-NB	2.22	111.06	109.47
3	C	201	HNI	C1A-NA-C4A	-2.21	101.08	105.25
3	C	201	HNI	CHA-C4D-C3D	-2.21	120.46	125.30
4	D	201	HEM	C2A-C1A-NA	2.18	112.57	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	201	HEM	CAD-C3D-C2D	-2.17	123.80	127.87
4	B	201	HEM	CHD-C4C-NC	2.17	126.81	124.45
6	B	203	IHP	O14-C4-C5	-2.16	104.17	108.76
4	B	201	HEM	C4A-NA-C1A	-2.16	102.31	105.82
4	B	201	HEM	CHA-C1A-C2A	-2.14	120.62	125.30
4	B	201	HEM	CHD-C1D-C2D	-2.12	121.68	125.03
3	C	201	HNI	CBD-CAD-C3D	-2.12	106.67	112.53
4	D	201	HEM	C3D-C4D-ND	2.12	112.49	110.17
6	B	203	IHP	C3-C2-C1	2.12	115.07	110.43
3	C	201	HNI	CHB-C1B-C2B	-2.11	121.09	125.49
4	B	201	HEM	O2A-CGA-CBA	2.11	120.65	114.00
4	D	201	HEM	CHD-C4C-C3C	-2.10	121.67	125.21
3	A	201	HNI	C1A-C2A-C3A	-2.08	103.86	106.89
4	B	201	HEM	C1A-CHA-C4D	-2.08	121.36	126.25
4	B	201	HEM	CAD-C3D-C4D	2.08	128.32	124.70
3	C	201	HNI	C4C-C3C-C2C	-2.07	105.38	107.28
3	A	201	HNI	O2A-CGA-CBA	2.06	120.50	114.00
3	C	201	HNI	O2D-CGD-CBD	2.06	120.50	114.00
4	B	201	HEM	CAA-CBA-CGA	-2.05	108.22	113.67
4	D	201	HEM	CAC-C3C-C4C	-2.03	119.98	124.82
3	C	201	HNI	C1D-CHD-C4C	-2.03	121.48	126.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	201	HNI	NB
3	C	201	HNI	NB

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	201	HNI	C2B-C3B-CAB-CBB
6	B	203	IHP	C2-C1-O11-P1
6	B	203	IHP	C6-C1-O11-P1
6	B	203	IHP	C1-C2-O12-P2
6	B	203	IHP	C3-C2-O12-P2
4	B	201	HEM	C2C-C3C-CAC-CBC
6	B	203	IHP	C5-O15-P5-O25
4	B	201	HEM	C3D-CAD-CBD-CGD
3	A	201	HNI	CAA-CBA-CGA-O2A
3	A	201	HNI	CAA-CBA-CGA-O1A
4	B	201	HEM	C4C-C3C-CAC-CBC

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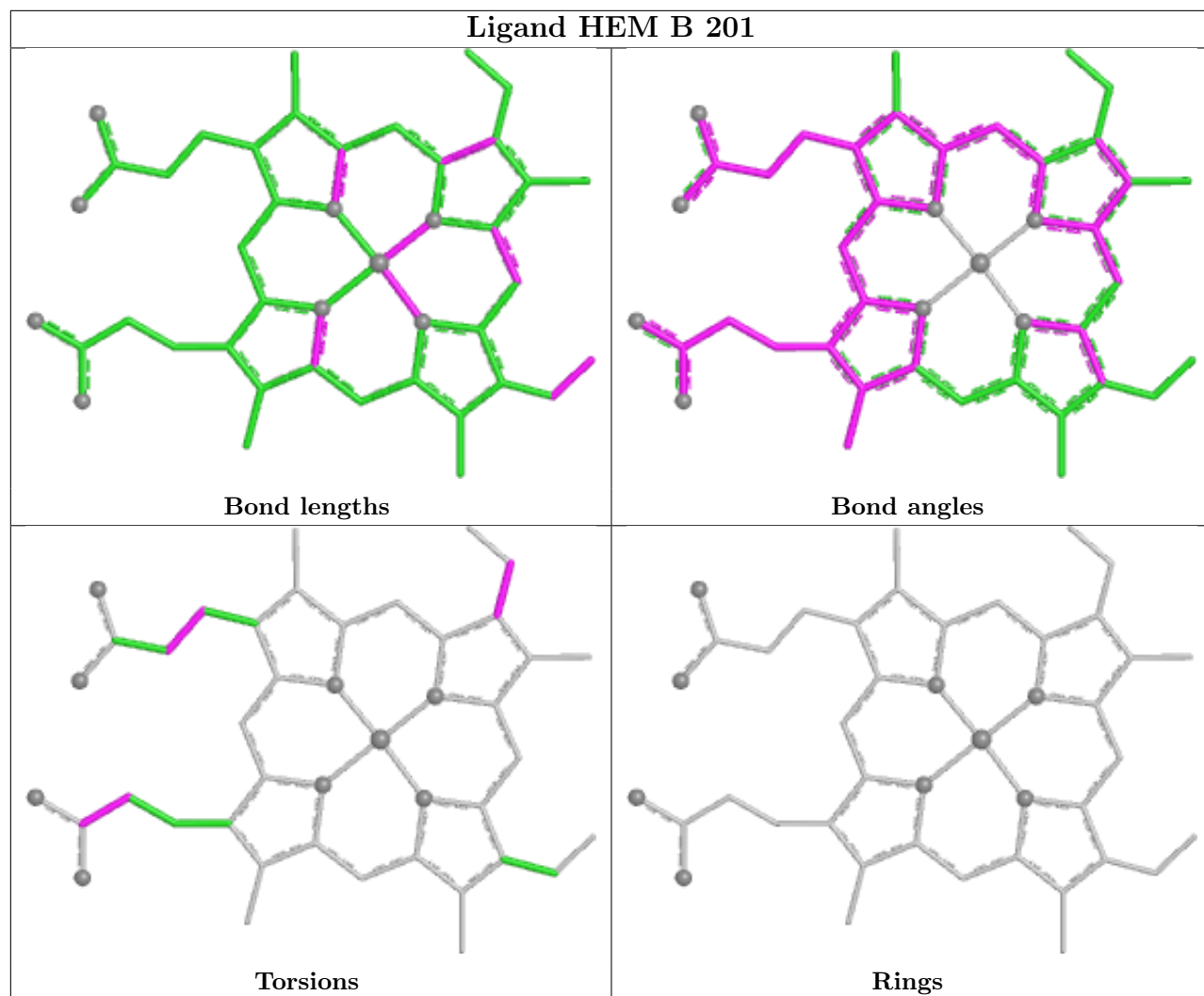
Mol	Chain	Res	Type	Atoms
6	B	203	IHP	C6-O16-P6-O46
3	A	201	HNI	CAD-CBD-CGD-O1D
4	D	201	HEM	CAD-CBD-CGD-O1D
4	D	201	HEM	CAD-CBD-CGD-O2D
3	A	201	HNI	CAD-CBD-CGD-O2D
4	B	201	HEM	CAA-CBA-CGA-O2A
4	D	201	HEM	C2B-C3B-CAB-CBB
3	C	201	HNI	CAD-CBD-CGD-O2D
4	B	201	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

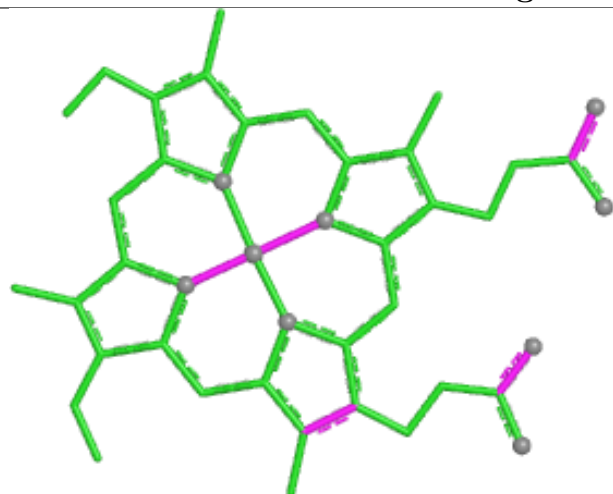
3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	201	HEM	3	0
4	D	201	HEM	0	1
6	B	203	IHP	5	0

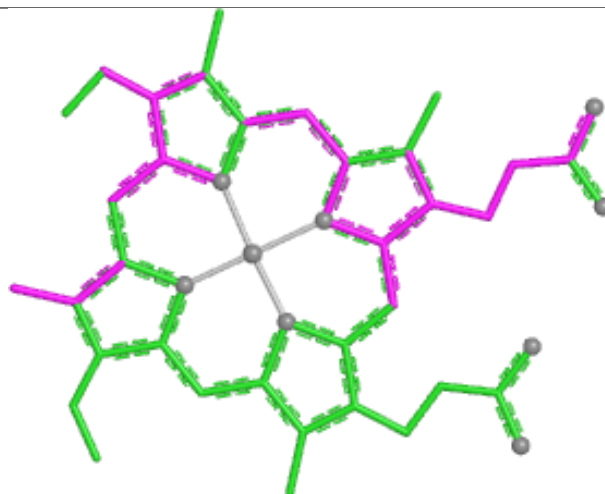
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



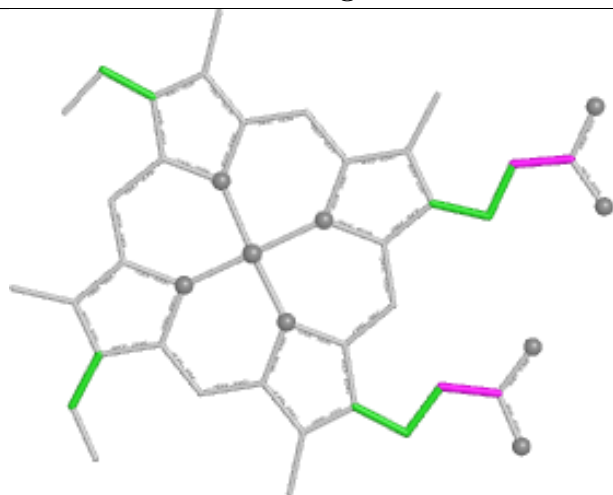
Ligand HNI A 201



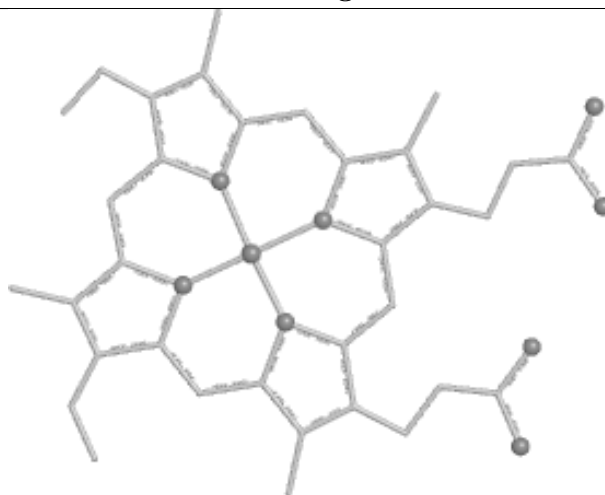
Bond lengths



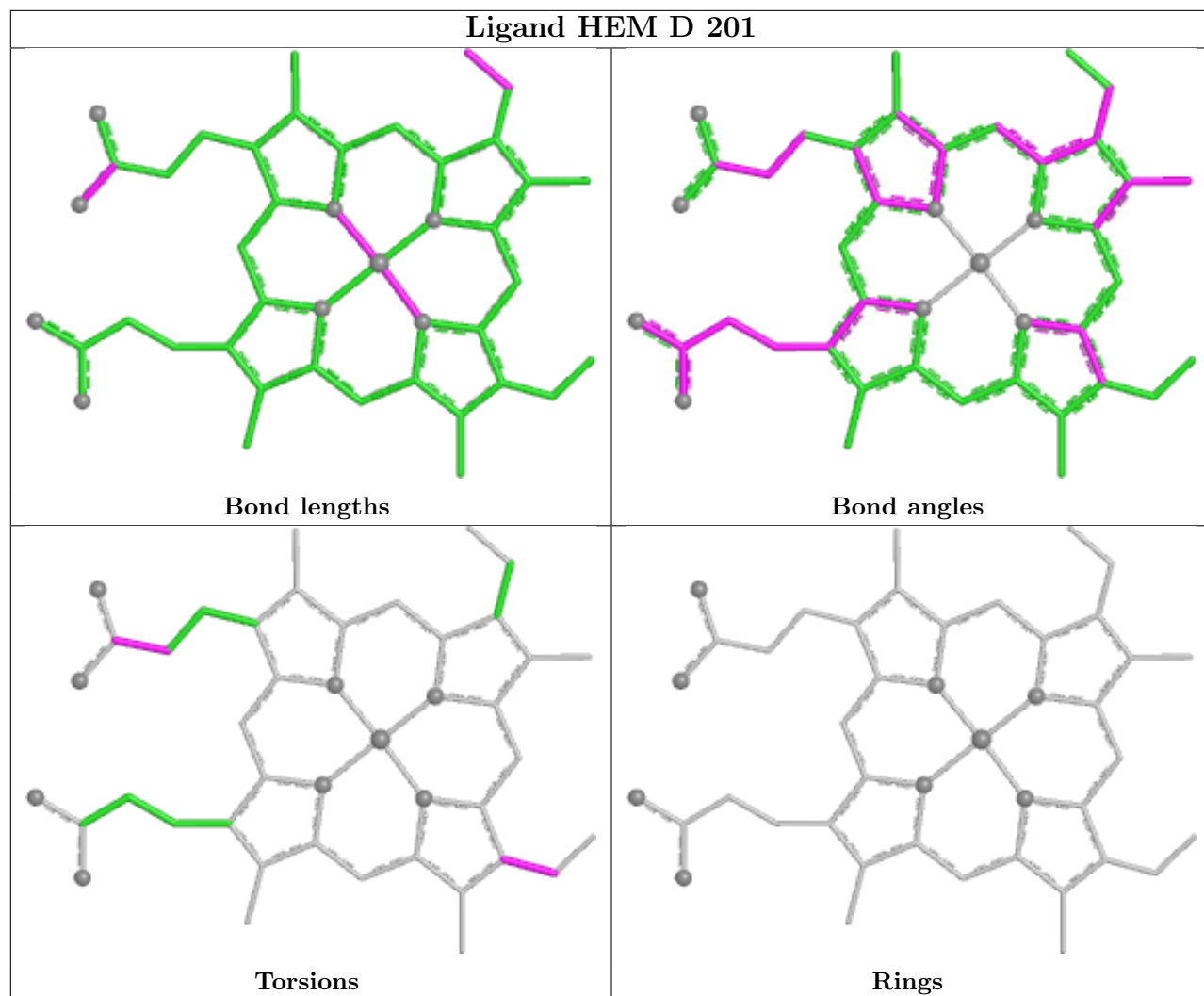
Bond angles



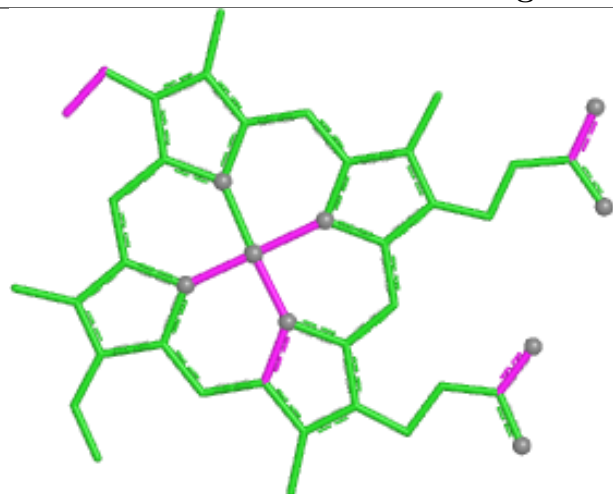
Torsions



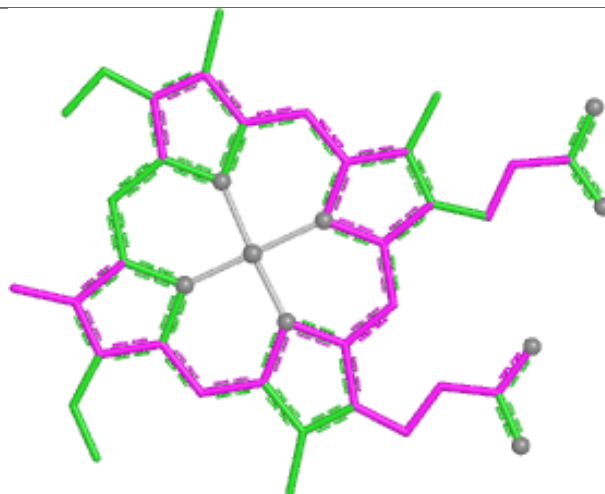
Rings



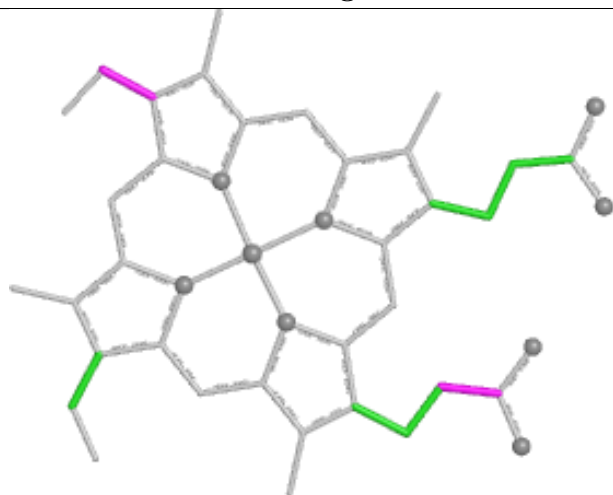
Ligand HNI C 201



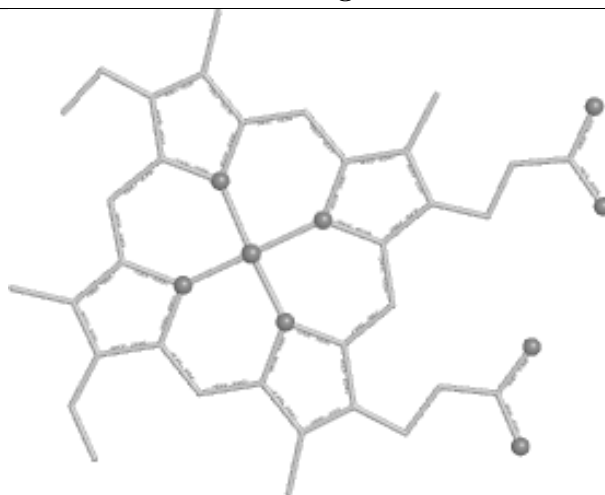
Bond lengths



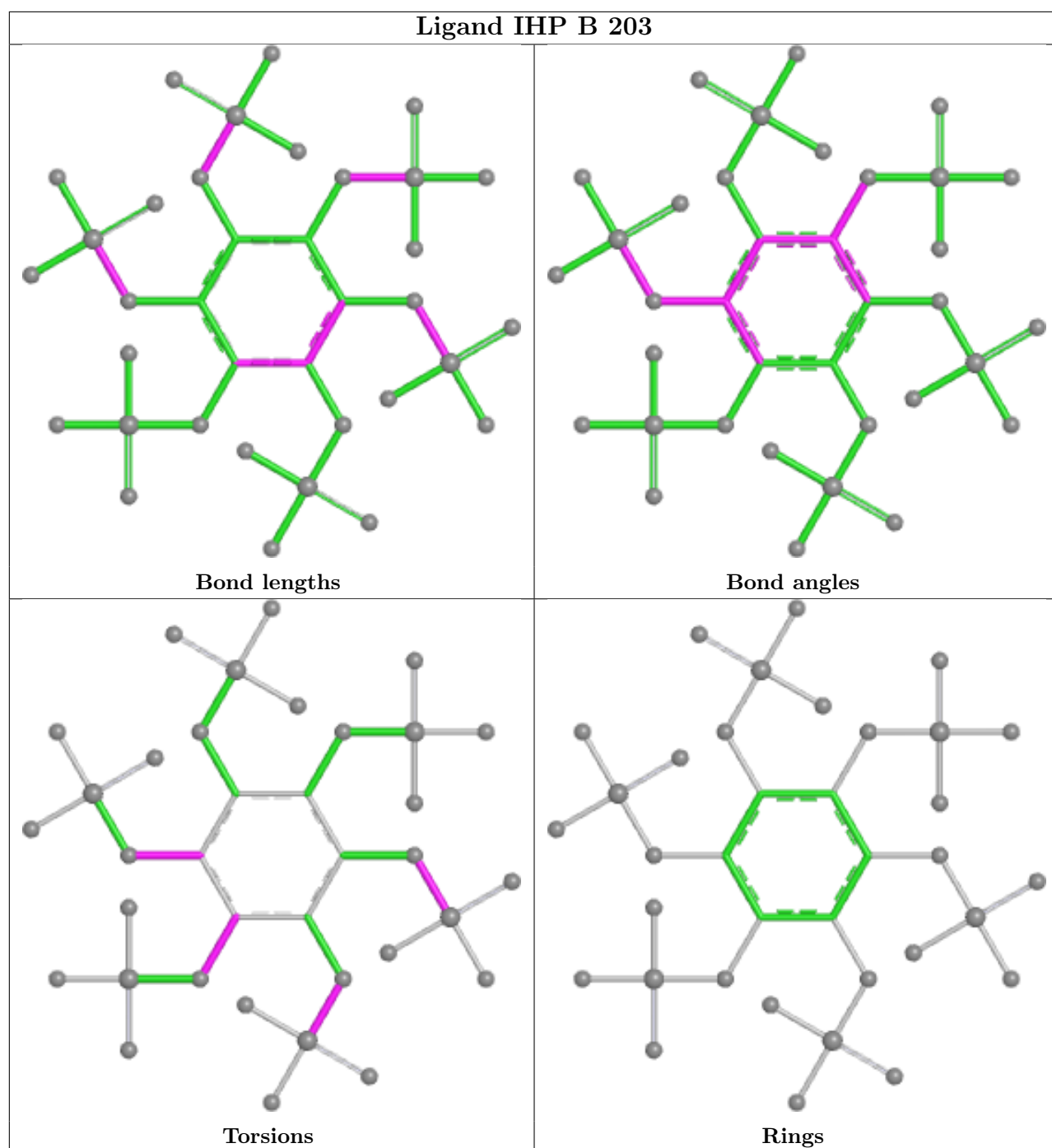
Bond angles



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 [i](#)

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.