



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:01 AM UTC

PDB ID : 1PRH / pdb_00001prh
Title : THE X-RAY CRYSTAL STRUCTURE OF THE MEMBRANE PROTEIN
PROSTAGLANDIN H2 SYNTHASE-1
Authors : Picot, D.; Loll, P.J.; Garavito, R.M.
Deposited on : 1994-03-07
Resolution : 3.50 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)	:	2.49

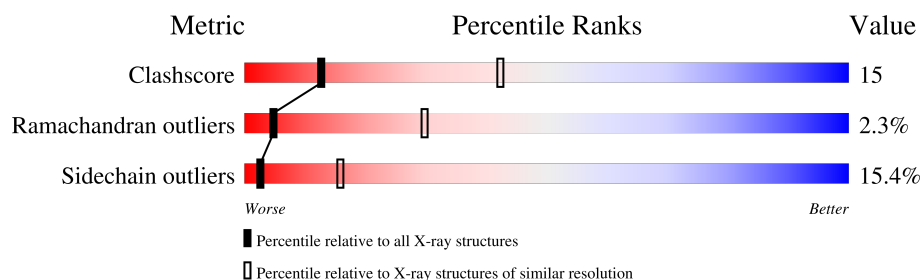
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)

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	554	54% 33% 10% .
1	B	554	54% 35% 9% .

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.

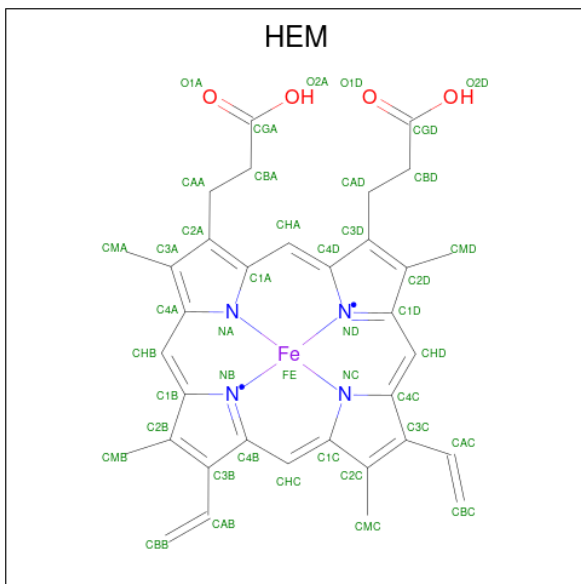
- Molecule 1 is a protein called PROSTAGLANDIN H2 SYNTHASE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total 4503	C 2919	N 762	O 794	S 28	0	0	0
1	B	554	Total 4503	C 2919	N 762	O 794	S 28	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	LEU	MET	conflict	UNP P05979
A	310	GLN	ASN	conflict	UNP P05979
A	333	LYS	ARG	conflict	UNP P05979
B	92	LEU	MET	conflict	UNP P05979
B	310	GLN	ASN	conflict	UNP P05979
B	333	LYS	ARG	conflict	UNP P05979

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



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

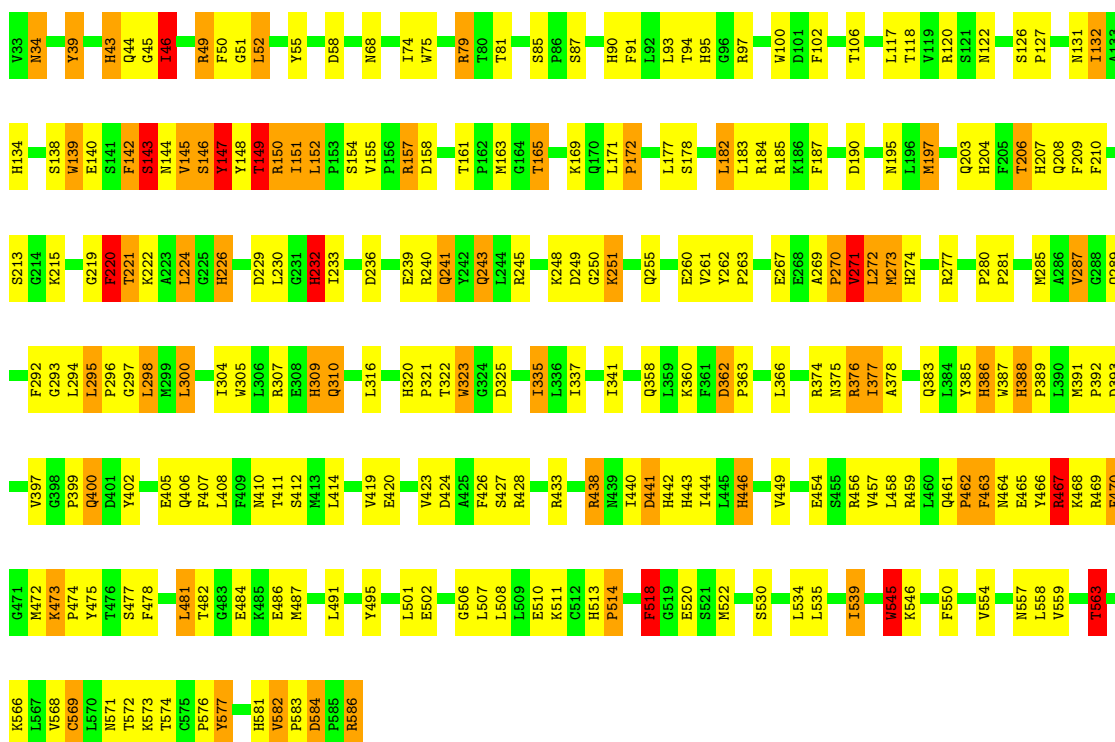
3 Residue-property plots [i](#)

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

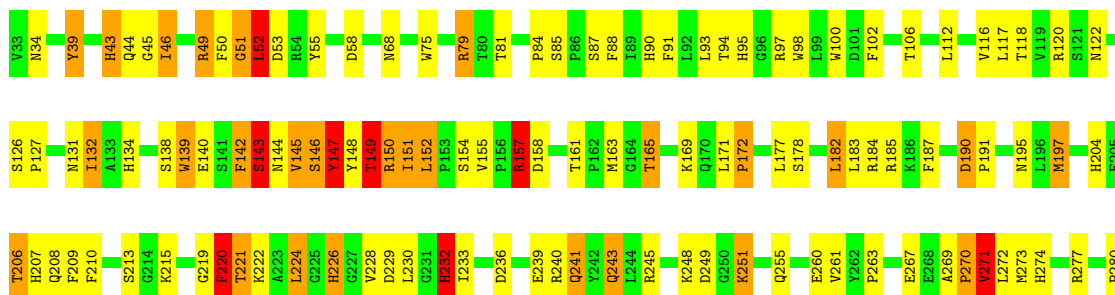
• Molecule 1: PROSTAGLANDIN H2 SYNTHASE-1

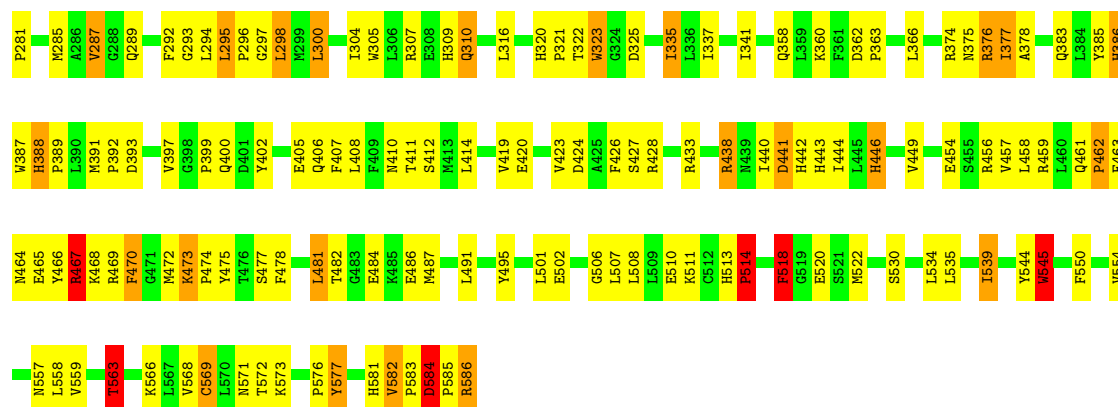
Chain A: 



• Molecule 1: PROSTAGLANDIN H2 SYNTHASE-1

Chain B: 





4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	99.40Å 210.30Å 233.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.267 , 0.316	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9092	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: 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	1.13	9/4642 (0.2%)	1.96	170/6299 (2.7%)
1	B	1.16	8/4642 (0.2%)	1.97	165/6299 (2.6%)
All	All	1.14	17/9284 (0.2%)	1.96	335/12598 (2.7%)

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	2
1	B	0	2
All	All	0	4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	462	PRO	C-N	-10.46	1.20	1.33
1	A	462	PRO	C-N	-10.21	1.20	1.33
1	B	477	SER	C-N	-6.93	1.24	1.34
1	A	477	SER	C-N	-6.70	1.24	1.34
1	A	95	HIS	CG-CD2	6.13	1.42	1.35
1	B	139	TRP	NE1-CE2	-5.77	1.31	1.37
1	B	95	HIS	CB-CG	5.63	1.58	1.50
1	B	95	HIS	CG-CD2	5.59	1.42	1.35
1	A	139	TRP	NE1-CE2	-5.40	1.31	1.37
1	B	293	GLY	C-N	-5.40	1.27	1.33
1	A	46	ILE	CA-CB	5.32	1.60	1.54
1	B	157	ARG	NE-CZ	5.29	1.38	1.33
1	A	95	HIS	CB-CG	5.19	1.57	1.50
1	B	545	TRP	CG-CD2	-5.12	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	457	VAL	C-N	-5.11	1.27	1.33
1	A	157	ARG	NE-CZ	5.03	1.38	1.33
1	A	293	GLY	C-N	-5.02	1.27	1.33

All (335) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	HIS	CA-CB-CG	21.00	134.80	113.80
1	B	95	HIS	CA-CB-CG	20.66	134.46	113.80
1	A	143	SER	O-C-N	-18.47	97.61	122.36
1	B	143	SER	O-C-N	-18.22	97.94	122.36
1	A	293	GLY	CA-C-N	14.37	142.38	120.82
1	A	293	GLY	C-N-CA	14.37	142.38	120.82
1	B	293	GLY	CA-C-N	14.35	142.35	120.82
1	B	293	GLY	C-N-CA	14.35	142.35	120.82
1	B	386	HIS	CA-CB-CG	-12.57	101.23	113.80
1	A	386	HIS	CA-CB-CG	-12.52	101.28	113.80
1	A	142	PHE	CA-CB-CG	-10.71	103.09	113.80
1	B	147	TYR	N-CA-C	10.24	126.30	114.62
1	B	142	PHE	CA-CB-CG	-10.21	103.59	113.80
1	A	147	TYR	N-CA-C	9.95	125.97	114.62
1	A	232	HIS	CA-CB-CG	9.86	123.66	113.80
1	B	232	HIS	CA-CB-CG	9.81	123.61	113.80
1	A	229	ASP	N-CA-C	-9.36	94.88	109.76
1	B	229	ASP	N-CA-C	-9.15	95.22	109.76
1	A	581	HIS	CB-CG-CD2	-8.90	119.63	131.20
1	A	229	ASP	CA-CB-CG	8.88	121.48	112.60
1	B	581	HIS	CB-CG-CD2	-8.83	119.72	131.20
1	B	486	GLU	O-C-N	-8.53	111.24	122.59
1	B	229	ASP	CA-CB-CG	8.53	121.13	112.60
1	B	207	HIS	CA-CB-CG	-8.44	105.36	113.80
1	A	486	GLU	O-C-N	-8.39	111.43	122.59
1	A	207	HIS	CA-CB-CG	-8.36	105.44	113.80
1	B	219	GLY	N-CA-C	-8.19	97.30	112.62
1	B	209	PHE	CA-CB-CG	8.11	121.91	113.80
1	A	209	PHE	CA-CB-CG	8.09	121.89	113.80
1	A	219	GLY	N-CA-C	-8.01	97.64	112.62
1	A	320	HIS	CA-CB-CG	7.91	121.71	113.80
1	A	132	ILE	CB-CA-C	-7.87	101.73	112.04
1	A	260	GLU	N-CA-C	7.86	122.09	110.46
1	B	320	HIS	CA-CB-CG	7.84	121.64	113.80
1	A	146	SER	N-CA-C	-7.72	100.69	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	260	GLU	N-CA-C	7.72	121.89	110.46
1	B	146	SER	N-CA-C	-7.61	100.85	111.81
1	A	584	ASP	CA-CB-CG	7.56	120.16	112.60
1	A	149	THR	CA-CB-OG1	-7.55	98.27	109.60
1	B	132	ILE	CB-CA-C	-7.55	102.15	112.04
1	B	226	HIS	N-CA-C	7.55	121.86	111.90
1	A	226	HIS	N-CA-C	7.52	121.83	111.90
1	B	120	ARG	NE-CZ-NH2	-7.51	112.44	119.20
1	B	584	ASP	CA-CB-CG	7.51	120.11	112.60
1	A	571	ASN	OD1-CG-ND2	-7.48	115.12	122.60
1	B	375	ASN	OD1-CG-ND2	-7.44	115.16	122.60
1	A	120	ARG	NE-CZ-NH2	-7.41	112.53	119.20
1	A	204	HIS	CA-CB-CG	7.40	121.20	113.80
1	B	149	THR	CA-CB-OG1	-7.38	98.53	109.60
1	B	571	ASN	OD1-CG-ND2	-7.37	115.23	122.60
1	B	545	TRP	CE2-CD2-CE3	7.37	126.17	118.80
1	B	387	TRP	CA-CB-CG	7.36	127.58	113.60
1	A	271	VAL	N-CA-CB	-7.30	99.18	111.23
1	A	375	ASN	OD1-CG-ND2	-7.30	115.30	122.60
1	B	271	VAL	N-CA-CB	-7.24	99.28	111.23
1	A	386	HIS	ND1-CG-CD2	7.20	113.30	106.10
1	B	94	THR	CA-C-O	7.20	128.68	121.20
1	A	387	TRP	CA-CB-CG	7.18	127.25	113.60
1	A	226	HIS	CB-CG-CD2	-7.18	121.87	131.20
1	B	386	HIS	ND1-CG-CD2	7.17	113.28	106.10
1	B	43	HIS	CG-CD2-NE2	-7.12	100.08	107.20
1	A	293	GLY	O-C-N	-7.12	114.52	122.28
1	B	243	GLN	CG-CD-NE2	7.12	127.07	116.40
1	B	204	HIS	CA-CB-CG	7.07	120.87	113.80
1	A	94	THR	CA-C-O	7.04	128.52	121.20
1	B	226	HIS	CB-CG-CD2	-7.04	122.05	131.20
1	A	134	HIS	CB-CG-CD2	-7.00	122.09	131.20
1	B	293	GLY	O-C-N	-6.99	114.83	122.24
1	A	219	GLY	O-C-N	-6.98	116.28	122.91
1	B	204	HIS	CB-CG-CD2	-6.88	122.26	131.20
1	A	243	GLN	CG-CD-NE2	6.88	126.71	116.40
1	A	271	VAL	N-CA-C	6.86	123.60	109.34
1	A	446	HIS	CB-CG-CD2	-6.84	122.31	131.20
1	A	325	ASP	N-CA-C	6.81	118.36	111.07
1	B	134	HIS	CB-CG-CD2	-6.80	122.35	131.20
1	A	43	HIS	CG-CD2-NE2	-6.78	100.42	107.20
1	A	563	THR	CA-CB-OG1	-6.78	99.43	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	446	HIS	CB-CG-CD2	-6.77	122.39	131.20
1	A	577	TYR	N-CA-C	-6.76	99.01	109.76
1	A	204	HIS	CB-CG-CD2	-6.74	122.44	131.20
1	A	545	TRP	CE2-CD2-CE3	6.74	125.53	118.80
1	B	85	SER	CA-C-N	6.72	126.23	119.24
1	B	85	SER	C-N-CA	6.72	126.23	119.24
1	B	219	GLY	O-C-N	-6.72	116.53	122.91
1	B	271	VAL	N-CA-C	6.69	123.25	109.34
1	B	325	ASP	N-CA-C	6.67	118.21	111.07
1	B	243	GLN	OE1-CD-NE2	-6.65	115.95	122.60
1	B	563	THR	CA-CB-OG1	-6.63	99.65	109.60
1	B	577	TYR	N-CA-C	-6.63	99.21	109.76
1	A	386	HIS	CB-CG-CD2	-6.62	122.59	131.20
1	B	152	LEU	CA-C-N	6.62	127.53	120.11
1	B	152	LEU	C-N-CA	6.62	127.53	120.11
1	B	386	HIS	CB-CG-CD2	-6.62	122.59	131.20
1	B	43	HIS	ND1-CG-CD2	6.58	112.68	106.10
1	B	387	TRP	CA-C-O	6.57	129.56	122.13
1	A	457	VAL	CA-C-N	6.56	131.10	120.60
1	A	457	VAL	C-N-CA	6.56	131.10	120.60
1	A	43	HIS	ND1-CG-CD2	6.56	112.66	106.10
1	B	386	HIS	CG-CD2-NE2	-6.56	100.64	107.20
1	B	457	VAL	CA-C-N	6.51	131.01	120.60
1	B	457	VAL	C-N-CA	6.51	131.01	120.60
1	A	386	HIS	CG-CD2-NE2	-6.47	100.73	107.20
1	B	581	HIS	ND1-CG-CD2	6.46	112.56	106.10
1	B	206	THR	N-CA-CB	-6.46	99.94	110.14
1	B	569	CYS	CA-CB-SG	-6.44	99.59	114.40
1	B	295	LEU	CB-CA-C	-6.43	100.00	109.97
1	A	243	GLN	OE1-CD-NE2	-6.42	116.18	122.60
1	A	569	CYS	CA-CB-SG	-6.42	99.64	114.40
1	B	204	HIS	ND1-CG-CD2	6.41	112.51	106.10
1	B	442	HIS	CB-CG-CD2	-6.40	122.88	131.20
1	A	206	THR	N-CA-CB	-6.37	100.08	110.14
1	B	287	VAL	N-CA-C	6.36	122.57	109.34
1	B	229	ASP	O-C-N	-6.35	115.61	123.04
1	A	152	LEU	CA-C-N	6.34	127.21	120.11
1	A	152	LEU	C-N-CA	6.34	127.21	120.11
1	B	513	HIS	CA-C-N	6.34	127.76	119.84
1	B	513	HIS	C-N-CA	6.34	127.76	119.84
1	A	470	PHE	CA-CB-CG	-6.33	107.47	113.80
1	A	387	TRP	CA-C-O	6.33	129.28	122.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	ASP	CA-CB-CG	6.31	118.91	112.60
1	A	513	HIS	CA-C-N	6.29	127.70	119.84
1	A	513	HIS	C-N-CA	6.29	127.70	119.84
1	A	274	HIS	CB-CG-CD2	-6.27	123.05	131.20
1	A	581	HIS	ND1-CG-CD2	6.25	112.36	106.10
1	B	468	LYS	O-C-N	6.25	128.59	122.09
1	A	158	ASP	CA-CB-CG	6.23	118.83	112.60
1	A	85	SER	CA-C-N	6.22	125.71	119.24
1	A	85	SER	C-N-CA	6.22	125.71	119.24
1	B	149	THR	CA-CB-CG2	6.22	121.07	110.50
1	A	287	VAL	N-CA-C	6.21	122.26	109.34
1	B	274	HIS	CB-CG-CD2	-6.21	123.12	131.20
1	B	120	ARG	NE-CZ-NH1	6.20	127.70	121.50
1	A	149	THR	CA-CB-CG2	6.20	121.04	110.50
1	B	470	PHE	CA-CB-CG	-6.16	107.64	113.80
1	A	204	HIS	ND1-CG-CD2	6.15	112.25	106.10
1	A	442	HIS	CB-CG-CD2	-6.14	123.22	131.20
1	A	95	HIS	CG-CD2-NE2	-6.12	101.08	107.20
1	B	335	ILE	CB-CA-C	-6.11	104.15	111.97
1	B	150	ARG	N-CA-C	-6.09	100.26	109.95
1	B	34	ASN	OD1-CG-ND2	-6.09	116.51	122.60
1	A	335	ILE	CB-CA-C	-6.07	104.20	111.97
1	A	34	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	A	274	HIS	CG-CD2-NE2	-6.05	101.15	107.20
1	A	305	TRP	CG-CD2-CE3	6.05	139.95	133.90
1	A	131	ASN	CA-C-O	-6.04	114.81	121.28
1	A	518	PHE	CA-CB-CG	6.04	119.84	113.80
1	A	584	ASP	N-CA-C	6.04	123.15	109.81
1	A	150	ARG	N-CA-C	-6.03	100.07	109.72
1	B	95	HIS	CG-CD2-NE2	-6.02	101.18	107.20
1	B	387	TRP	N-CA-C	6.01	119.11	108.24
1	A	274	HIS	ND1-CG-CD2	6.00	112.11	106.10
1	A	120	ARG	NE-CZ-NH1	6.00	127.50	121.50
1	A	387	TRP	N-CA-C	6.00	119.11	108.24
1	A	387	TRP	N-CA-CB	-5.99	101.68	110.49
1	A	442	HIS	CG-CD2-NE2	-5.99	101.21	107.20
1	A	229	ASP	O-C-N	-5.97	116.05	123.04
1	A	513	HIS	ND1-CG-CD2	5.97	112.07	106.10
1	B	442	HIS	CG-CD2-NE2	-5.96	101.23	107.20
1	A	581	HIS	CG-CD2-NE2	-5.95	101.25	107.20
1	A	222	LYS	N-CA-C	-5.95	105.86	113.23
1	B	584	ASP	N-CA-C	5.93	122.92	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	ASP	CA-CB-CG	5.92	118.52	112.60
1	B	571	ASN	CB-CG-ND2	5.92	125.27	116.40
1	B	274	HIS	ND1-CG-CD2	5.90	112.00	106.10
1	A	236	ASP	CA-CB-CG	5.90	118.50	112.60
1	B	232	HIS	ND1-CG-CD2	5.89	111.99	106.10
1	B	43	HIS	CB-CG-CD2	-5.88	123.56	131.20
1	B	144	ASN	CB-CG-ND2	5.88	125.22	116.40
1	A	468	LYS	O-C-N	5.88	128.20	122.09
1	A	183	LEU	N-CA-C	5.87	118.84	110.10
1	A	571	ASN	CB-CG-ND2	5.85	125.18	116.40
1	A	90	HIS	CB-CG-CD2	-5.85	123.60	131.20
1	B	90	HIS	CB-CG-CD2	-5.84	123.60	131.20
1	B	518	PHE	CA-CB-CG	5.84	119.64	113.80
1	A	443	HIS	CA-CB-CG	5.83	119.63	113.80
1	B	183	LEU	N-CA-C	5.83	118.78	110.10
1	B	131	ASN	CA-C-O	-5.83	115.05	121.28
1	A	513	HIS	CB-CG-CD2	-5.81	123.65	131.20
1	B	151	ILE	CB-CG1-CD1	-5.81	101.60	113.80
1	A	134	HIS	N-CA-C	5.80	117.85	108.34
1	B	134	HIS	N-CA-C	5.80	117.85	108.34
1	B	274	HIS	CG-CD2-NE2	-5.80	101.40	107.20
1	B	222	LYS	N-CA-C	-5.79	106.05	113.23
1	A	513	HIS	CG-CD2-NE2	-5.78	101.42	107.20
1	A	144	ASN	CB-CG-ND2	5.77	125.05	116.40
1	B	581	HIS	CG-CD2-NE2	-5.76	101.44	107.20
1	B	387	TRP	N-CA-CB	-5.76	102.02	110.49
1	B	446	HIS	CG-CD2-NE2	-5.76	101.44	107.20
1	A	251	LYS	O-C-N	5.74	129.37	122.94
1	A	206	THR	CA-CB-OG1	-5.72	101.02	109.60
1	B	305	TRP	CB-CG-CD1	-5.71	118.33	126.90
1	A	43	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	A	138	SER	CA-C-N	-5.70	111.65	120.31
1	A	138	SER	C-N-CA	-5.70	111.65	120.31
1	A	309	HIS	CB-CG-CD2	-5.68	123.81	131.20
1	A	151	ILE	CB-CG1-CD1	-5.68	101.88	113.80
1	A	305	TRP	CB-CG-CD1	-5.67	118.39	126.90
1	B	443	HIS	CA-CB-CG	5.67	119.47	113.80
1	B	204	HIS	CG-CD2-NE2	-5.67	101.53	107.20
1	B	309	HIS	CB-CG-CD2	-5.67	123.83	131.20
1	B	305	TRP	CG-CD2-CE3	5.64	139.54	133.90
1	A	274	HIS	CA-CB-CG	-5.63	108.17	113.80
1	B	68	ASN	CA-CB-CG	5.62	118.22	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ASN	OD1-CG-ND2	-5.61	116.99	122.60
1	B	138	SER	CA-C-N	-5.61	111.78	120.31
1	B	138	SER	C-N-CA	-5.61	111.78	120.31
1	B	132	ILE	N-CA-CB	5.61	117.48	110.47
1	B	513	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	B	274	HIS	CA-CB-CG	-5.60	108.20	113.80
1	A	563	THR	CA-CB-CG2	5.58	119.99	110.50
1	A	91	PHE	CA-CB-CG	-5.58	108.22	113.80
1	A	251	LYS	CB-CG-CD	5.58	124.13	111.30
1	B	583	PRO	O-C-N	5.57	129.91	123.01
1	A	446	HIS	CG-CD2-NE2	-5.56	101.64	107.20
1	B	251	LYS	O-C-N	5.56	129.17	122.94
1	B	90	HIS	CG-CD2-NE2	-5.56	101.64	107.20
1	A	393	ASP	CA-CB-CG	5.55	118.15	112.60
1	B	232	HIS	CG-CD2-NE2	-5.55	101.65	107.20
1	B	206	THR	CA-CB-OG1	-5.54	101.29	109.60
1	A	388	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	B	446	HIS	ND1-CG-CD2	5.52	111.62	106.10
1	A	100	TRP	CG-CD2-CE3	5.52	139.42	133.90
1	A	295	LEU	CB-CA-C	-5.51	99.89	109.32
1	B	467	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	A	388	HIS	ND1-CE1-NE2	5.51	113.91	108.40
1	B	513	HIS	ND1-CG-CD2	5.50	111.61	106.10
1	B	251	LYS	CB-CG-CD	5.50	123.94	111.30
1	B	388	HIS	CB-CG-CD2	-5.50	124.06	131.20
1	A	446	HIS	ND1-CG-CD2	5.49	111.59	106.10
1	B	68	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	B	388	HIS	ND1-CE1-NE2	5.48	113.88	108.40
1	A	442	HIS	ND1-CG-CD2	5.46	111.56	106.10
1	A	583	PRO	O-C-N	5.45	129.77	123.01
1	A	90	HIS	CG-CD2-NE2	-5.44	101.76	107.20
1	A	269	ALA	CA-C-N	5.44	126.64	119.84
1	A	269	ALA	C-N-CA	5.44	126.64	119.84
1	A	132	ILE	N-CA-CB	5.43	117.25	110.47
1	A	309	HIS	ND1-CG-CD2	5.42	111.52	106.10
1	B	165	THR	CA-CB-OG1	-5.42	101.47	109.60
1	A	203	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	B	144	ASN	N-CA-C	-5.41	98.92	108.23
1	A	309	HIS	CG-CD2-NE2	-5.41	101.79	107.20
1	B	563	THR	CA-CB-CG2	5.41	119.69	110.50
1	B	39	TYR	CA-C-N	5.40	124.92	119.19
1	B	39	TYR	C-N-CA	5.40	124.92	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	443	HIS	ND1-CG-CD2	5.40	111.50	106.10
1	B	442	HIS	ND1-CG-CD2	5.40	111.50	106.10
1	A	467	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	B	269	ALA	CA-C-N	5.39	126.58	119.84
1	B	269	ALA	C-N-CA	5.39	126.58	119.84
1	B	90	HIS	ND1-CG-CD2	5.38	111.48	106.10
1	B	309	HIS	ND1-CG-CD2	5.37	111.47	106.10
1	B	441	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	513	HIS	CG-CD2-NE2	-5.37	101.83	107.20
1	A	144	ASN	N-CA-C	-5.36	99.00	108.23
1	B	309	HIS	CG-CD2-NE2	-5.36	101.84	107.20
1	A	337	ILE	N-CA-C	-5.35	105.28	110.42
1	A	377	ILE	N-CA-CB	5.35	116.36	110.53
1	B	220	PHE	N-CA-C	5.35	122.19	110.80
1	A	68	ASN	CA-CB-CG	5.34	117.94	112.60
1	B	557	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	A	213	SER	N-CA-C	5.31	117.76	111.33
1	B	122	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	A	122	ASN	CB-CG-ND2	5.29	124.34	116.40
1	A	145	VAL	N-CA-CB	-5.29	102.51	111.23
1	B	145	VAL	N-CA-CB	-5.26	102.55	111.23
1	B	91	PHE	CA-CB-CG	-5.25	108.55	113.80
1	A	514	PRO	CA-N-CD	-5.25	104.65	112.00
1	B	161	THR	N-CA-C	-5.24	103.34	110.36
1	A	143	SER	CA-C-N	5.24	130.66	122.17
1	A	143	SER	C-N-CA	5.24	130.66	122.17
1	B	75	TRP	CE2-CD2-CG	-5.24	100.91	107.20
1	A	232	HIS	ND1-CG-CD2	5.23	111.33	106.10
1	B	377	ILE	N-CA-CB	5.22	116.22	110.53
1	A	442	HIS	N-CA-C	5.22	118.43	111.75
1	B	144	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	A	220	PHE	N-CA-C	5.21	121.89	110.80
1	B	514	PRO	CA-N-CD	-5.21	104.71	112.00
1	A	68	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	A	39	TYR	CA-C-N	5.20	124.70	119.19
1	A	39	TYR	C-N-CA	5.20	124.70	119.19
1	B	100	TRP	CG-CD2-CE3	5.17	139.07	133.90
1	B	122	ASN	CB-CG-ND2	5.17	124.15	116.40
1	A	443	HIS	ND1-CG-CD2	5.16	111.26	106.10
1	A	75	TRP	CE2-CD2-CG	-5.15	101.02	107.20
1	A	204	HIS	CG-CD2-NE2	-5.15	102.05	107.20
1	A	557	ASN	OD1-CG-ND2	-5.14	117.46	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	393	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	546	LYS	N-CA-C	-5.13	101.39	109.50
1	B	134	HIS	CG-CD2-NE2	-5.13	102.07	107.20
1	A	539	ILE	CA-CB-CG1	-5.12	101.69	110.40
1	B	232	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	B	127	PRO	CA-C-N	5.11	125.38	119.92
1	B	127	PRO	C-N-CA	5.11	125.38	119.92
1	B	221	THR	N-CA-C	-5.10	101.39	109.76
1	B	45	GLY	N-CA-C	-5.10	106.01	112.54
1	B	337	ILE	N-CA-C	-5.10	105.53	110.42
1	A	134	HIS	CG-CD2-NE2	-5.09	102.11	107.20
1	A	362	ASP	CA-C-N	5.09	125.38	119.47
1	A	362	ASP	C-N-CA	5.09	125.38	119.47
1	A	441	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	127	PRO	CA-C-N	5.08	125.36	119.92
1	A	127	PRO	C-N-CA	5.08	125.36	119.92
1	A	358	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	B	190	ASP	CA-C-N	5.07	124.68	119.05
1	B	190	ASP	C-N-CA	5.07	124.68	119.05
1	B	442	HIS	N-CA-C	5.07	118.24	111.75
1	A	232	HIS	CG-CD2-NE2	-5.06	102.14	107.20
1	A	320	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	A	165	THR	CA-CB-OG1	-5.06	102.01	109.60
1	B	143	SER	CA-C-N	5.06	130.37	122.17
1	B	143	SER	C-N-CA	5.06	130.37	122.17
1	A	443	HIS	CG-CD2-NE2	-5.05	102.15	107.20
1	B	224	LEU	N-CA-C	-5.05	103.87	110.53
1	B	539	ILE	CA-CB-CG1	-5.05	101.82	110.40
1	B	98	TRP	CE2-CD2-CE3	5.04	123.84	118.80
1	B	320	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	A	161	THR	N-CA-C	-5.04	103.61	110.36
1	B	213	SER	N-CA-C	5.03	117.42	111.33
1	A	463	PHE	O-C-N	5.03	127.46	122.03
1	A	262	TYR	CA-C-N	5.02	125.55	120.38
1	A	262	TYR	C-N-CA	5.02	125.55	120.38
1	A	221	THR	N-CA-C	-5.02	101.53	109.76
1	A	34	ASN	N-CA-CB	5.02	119.30	110.37
1	A	224	LEU	N-CA-C	-5.02	103.91	110.53
1	B	358	GLN	OE1-CD-NE2	-5.02	117.58	122.60
1	A	400	GLN	OE1-CD-NE2	-5.02	117.58	122.60
1	B	323	TRP	CE2-CD2-CG	-5.01	101.18	107.20
1	B	513	HIS	N-CA-C	-5.01	103.46	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	443	HIS	CG-CD2-NE2	-5.01	102.19	107.20
1	A	323	TRP	CB-CG-CD1	-5.01	119.39	126.90
1	A	45	GLY	N-CA-C	-5.01	106.13	112.54
1	A	190	ASP	CA-C-N	5.00	124.60	119.05
1	A	190	ASP	C-N-CA	5.00	124.60	119.05
1	A	90	HIS	ND1-CG-CD2	5.00	111.10	106.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	SER	Mainchain
1	A	584	ASP	Peptide
1	B	143	SER	Mainchain
1	B	584	ASP	Peptide

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	4503	0	4412	137	0
1	B	4503	0	4412	141	0
2	A	43	0	30	4	0
2	B	43	0	30	4	0
All	All	9092	0	8884	274	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 15.

All (274) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:PHE:O	1:A:142:PHE:CD1	1.98	1.15
1:B:142:PHE:O	1:B:142:PHE:CD1	1.98	1.15
1:A:142:PHE:CD1	1:A:142:PHE:C	2.30	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:PHE:CD1	1:B:142:PHE:C	2.30	1.08
1:B:462:PRO:HG2	1:B:465:GLU:HG2	1.36	1.06
1:A:462:PRO:HG2	1:A:465:GLU:HG2	1.36	1.03
1:A:462:PRO:HG2	1:A:465:GLU:CG	2.06	0.84
1:B:462:PRO:HG2	1:B:465:GLU:CG	2.07	0.83
1:A:461:GLN:HB3	1:A:462:PRO:HD2	1.59	0.82
1:B:461:GLN:HB3	1:B:462:PRO:HD2	1.60	0.82
1:B:292:PHE:CD1	1:B:298:LEU:HG	2.18	0.79
1:B:481:LEU:HD11	1:B:501:LEU:HD21	1.65	0.78
1:A:292:PHE:CD1	1:A:298:LEU:HG	2.18	0.78
1:A:481:LEU:HD11	1:A:501:LEU:HD21	1.66	0.77
1:A:142:PHE:C	1:A:142:PHE:HD1	1.93	0.77
1:B:142:PHE:C	1:B:142:PHE:HD1	1.92	0.76
1:B:463:PHE:HE2	1:B:506:GLY:C	1.95	0.75
1:A:463:PHE:HE2	1:A:506:GLY:C	1.95	0.74
1:A:482:THR:O	1:A:511:LYS:HB3	1.89	0.72
1:A:464:ASN:HA	1:A:467:ARG:HB2	1.72	0.72
1:B:482:THR:O	1:B:511:LYS:HB3	1.89	0.71
1:B:464:ASN:HA	1:B:467:ARG:HB2	1.72	0.70
1:B:463:PHE:CE2	1:B:506:GLY:C	2.70	0.70
1:A:185:ARG:HH21	1:A:438:ARG:HD2	1.57	0.70
1:A:463:PHE:HE2	1:A:507:LEU:N	1.89	0.69
1:B:463:PHE:HE2	1:B:507:LEU:N	1.89	0.69
1:B:185:ARG:HH21	1:B:438:ARG:HD2	1.56	0.69
1:A:463:PHE:CE2	1:A:506:GLY:C	2.70	0.69
1:A:184:ARG:HD2	1:A:187:PHE:HA	1.76	0.68
1:B:184:ARG:HD2	1:B:187:PHE:HA	1.76	0.67
1:A:463:PHE:O	1:A:466:TYR:HB2	1.96	0.66
1:B:463:PHE:O	1:B:466:TYR:HB2	1.96	0.66
1:A:157:ARG:HA	1:A:459:ARG:NH1	2.12	0.65
1:B:157:ARG:HA	1:B:459:ARG:NH1	2.12	0.64
1:B:172:PRO:HB2	1:B:177:LEU:HD11	1.79	0.64
1:B:391:MET:HG3	2:B:601:HEM:HMC3	1.80	0.64
1:A:391:MET:HG3	2:A:601:HEM:HMC3	1.80	0.63
1:B:464:ASN:ND2	1:B:474:PRO:HB2	2.13	0.63
1:A:321:PRO:HD2	1:B:51:GLY:HA2	1.79	0.63
1:A:172:PRO:HB2	1:A:177:LEU:HD11	1.79	0.62
1:A:464:ASN:ND2	1:A:474:PRO:HB2	2.13	0.62
1:B:304:ILE:HD13	1:B:568:VAL:HG22	1.81	0.62
1:A:463:PHE:CD2	1:A:506:GLY:HA3	2.35	0.62
1:A:241:GLN:NE2	1:A:245:ARG:HD2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:VAL:HG12	1:B:402:TYR:CE2	2.35	0.62
1:B:463:PHE:CD2	1:B:506:GLY:HA3	2.36	0.61
1:B:241:GLN:NE2	1:B:245:ARG:HD2	2.15	0.61
1:A:304:ILE:HD13	1:A:568:VAL:HG22	1.81	0.61
1:A:397:VAL:HG12	1:A:402:TYR:CE2	2.35	0.61
1:B:397:VAL:HG12	1:B:402:TYR:HE2	1.66	0.61
1:A:461:GLN:HB3	1:A:462:PRO:CD	2.31	0.60
1:B:195:ASN:HB3	1:B:582:VAL:HG23	1.84	0.60
1:A:145:VAL:HG13	1:A:224:LEU:HD23	1.84	0.60
1:A:195:ASN:HB3	1:A:582:VAL:HG23	1.84	0.60
1:B:145:VAL:HG13	1:B:224:LEU:HD23	1.84	0.59
1:B:208:GLN:HE22	1:B:230:LEU:HD23	1.68	0.58
1:A:397:VAL:HG12	1:A:402:TYR:HE2	1.67	0.58
1:A:49:ARG:HG3	1:A:49:ARG:HH11	1.69	0.56
1:A:208:GLN:HE22	1:A:230:LEU:HD23	1.68	0.56
1:B:461:GLN:CB	1:B:462:PRO:HD2	2.31	0.56
1:A:461:GLN:CB	1:A:462:PRO:HD2	2.31	0.56
1:B:49:ARG:HG3	1:B:49:ARG:HH11	1.69	0.56
1:B:563:THR:HG22	1:B:566:LYS:H	1.70	0.56
1:A:51:GLY:HA2	1:B:321:PRO:HD2	1.88	0.56
1:A:563:THR:HG22	1:A:566:LYS:H	1.71	0.55
1:B:241:GLN:HE22	1:B:245:ARG:HH11	1.54	0.55
1:B:461:GLN:HB3	1:B:462:PRO:CD	2.31	0.55
1:B:240:ARG:HH22	1:B:273:MET:HE2	1.72	0.55
1:A:241:GLN:HE22	1:A:245:ARG:HH11	1.54	0.54
1:A:389:PRO:HG3	1:A:440:ILE:HG12	1.89	0.54
1:A:481:LEU:CD1	1:A:501:LEU:HD21	2.37	0.54
1:B:389:PRO:HG3	1:B:440:ILE:HG12	1.89	0.54
1:B:481:LEU:C	1:B:481:LEU:CD2	2.81	0.54
1:A:285:MET:HE1	1:A:414:LEU:HD23	1.89	0.54
1:B:46:ILE:HG23	1:B:58:ASP:HB3	1.89	0.54
1:A:586:ARG:HA	1:A:586:ARG:NE	2.22	0.54
1:A:46:ILE:HG23	1:A:58:ASP:HB3	1.90	0.53
1:A:481:LEU:C	1:A:481:LEU:CD2	2.81	0.53
1:B:464:ASN:OD1	1:B:474:PRO:HA	2.08	0.53
1:B:586:ARG:HA	1:B:586:ARG:NE	2.23	0.53
1:B:285:MET:HE1	1:B:414:LEU:HD23	1.89	0.53
1:A:240:ARG:HH22	1:A:273:MET:HE2	1.73	0.53
1:A:569:CYS:HA	1:A:572:THR:HG22	1.90	0.53
1:B:518:PHE:CD2	1:B:522:MET:HG2	2.44	0.53
1:A:481:LEU:CD1	1:A:501:LEU:CD2	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:PHE:CD2	1:A:522:MET:HG2	2.43	0.53
1:B:481:LEU:CD1	1:B:501:LEU:CD2	2.87	0.52
1:A:464:ASN:OD1	1:A:474:PRO:HA	2.08	0.52
1:A:586:ARG:HA	1:A:586:ARG:HE	1.75	0.52
1:B:146:SER:O	1:B:220:PHE:HA	2.09	0.52
1:A:464:ASN:ND2	1:A:474:PRO:CB	2.72	0.52
1:B:383:GLN:O	1:B:386:HIS:HB2	2.10	0.52
1:A:146:SER:O	1:A:220:PHE:HA	2.10	0.52
1:B:464:ASN:ND2	1:B:474:PRO:CB	2.72	0.52
1:B:495:TYR:OH	1:B:502:GLU:HG3	2.09	0.52
1:A:383:GLN:O	1:A:386:HIS:HB2	2.10	0.52
1:A:473:LYS:H	1:A:473:LYS:HD3	1.74	0.52
1:A:495:TYR:OH	1:A:502:GLU:HG3	2.09	0.52
1:B:569:CYS:HA	1:B:572:THR:HG22	1.91	0.52
1:B:473:LYS:H	1:B:473:LYS:HD3	1.74	0.51
1:A:232:HIS:CD2	1:A:233:ILE:HG13	2.45	0.51
1:B:142:PHE:O	1:B:142:PHE:CG	2.60	0.51
1:B:481:LEU:CD1	1:B:501:LEU:HD21	2.36	0.51
1:B:335:ILE:HD13	1:B:550:PHE:HD1	1.76	0.51
1:B:481:LEU:HD11	1:B:501:LEU:CD2	2.39	0.51
1:A:335:ILE:HD13	1:A:550:PHE:HD1	1.75	0.51
1:A:295:LEU:HB3	1:A:296:PRO:HD2	1.93	0.50
1:B:232:HIS:CD2	1:B:233:ILE:HG13	2.46	0.50
1:B:586:ARG:HA	1:B:586:ARG:HE	1.75	0.50
1:A:139:TRP:O	1:A:142:PHE:HB3	2.11	0.50
1:A:461:GLN:CB	1:A:462:PRO:CD	2.89	0.50
1:B:462:PRO:CG	1:B:465:GLU:HG2	2.26	0.50
1:A:79:ARG:HH11	1:A:79:ARG:HG2	1.77	0.50
1:B:464:ASN:HD21	1:B:475:TYR:N	2.09	0.50
1:B:295:LEU:HB3	1:B:296:PRO:HD2	1.93	0.50
1:A:481:LEU:HD11	1:A:501:LEU:CD2	2.41	0.50
1:B:139:TRP:O	1:B:142:PHE:HB3	2.11	0.50
1:A:197:MET:HE3	1:A:423:VAL:HA	1.93	0.49
1:A:463:PHE:CE2	1:A:506:GLY:HA3	2.46	0.49
1:A:464:ASN:HD21	1:A:475:TYR:N	2.09	0.49
1:B:208:GLN:HB3	1:B:232:HIS:ND1	2.27	0.49
1:A:49:ARG:HG3	1:A:49:ARG:NH1	2.28	0.49
1:B:49:ARG:HG3	1:B:49:ARG:NH1	2.28	0.49
1:B:197:MET:HE3	1:B:423:VAL:HA	1.93	0.49
1:B:461:GLN:CB	1:B:462:PRO:CD	2.89	0.49
1:A:185:ARG:NH2	1:A:438:ARG:HH11	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLN:HB3	1:A:232:HIS:ND1	2.28	0.49
1:B:463:PHE:CE2	1:B:506:GLY:HA3	2.47	0.49
1:A:406:GLN:O	1:A:410:ASN:HB2	2.12	0.49
1:B:467:ARG:HH12	1:B:473:LYS:NZ	2.11	0.49
1:A:43:HIS:O	1:A:44:GLN:HG2	2.13	0.49
1:B:79:ARG:HG2	1:B:79:ARG:HH11	1.78	0.49
1:B:185:ARG:NH2	1:B:438:ARG:HH11	2.10	0.49
1:B:241:GLN:HE21	1:B:245:ARG:HD2	1.78	0.49
1:A:255:GLN:HG2	1:A:263:PRO:O	2.13	0.48
1:A:467:ARG:HH12	1:A:473:LYS:NZ	2.11	0.48
1:B:406:GLN:O	1:B:410:ASN:HB2	2.12	0.48
1:A:292:PHE:CG	1:A:298:LEU:HG	2.48	0.48
1:B:296:PRO:HG2	1:B:407:PHE:CE1	2.49	0.48
1:B:255:GLN:HG2	1:B:263:PRO:O	2.14	0.48
1:B:292:PHE:CG	1:B:298:LEU:HG	2.48	0.48
1:A:206:THR:HG23	1:A:210:PHE:HD2	1.79	0.48
1:A:240:ARG:HG3	1:A:271:VAL:HG22	1.95	0.48
1:A:481:LEU:HD12	1:A:501:LEU:HD22	1.96	0.48
1:B:43:HIS:O	1:B:44:GLN:HG2	2.13	0.48
1:B:481:LEU:HD12	1:B:501:LEU:HD22	1.96	0.48
1:A:241:GLN:HE21	1:A:245:ARG:HD2	1.78	0.47
1:A:296:PRO:HG2	1:A:407:PHE:CE1	2.49	0.47
1:B:240:ARG:HG3	1:B:271:VAL:HG22	1.95	0.47
1:B:184:ARG:HA	1:B:438:ARG:O	2.14	0.47
1:A:462:PRO:CG	1:A:465:GLU:HG2	2.26	0.47
1:A:462:PRO:O	1:A:466:TYR:HD2	1.97	0.47
1:A:294:LEU:HG	1:A:295:LEU:CD1	2.45	0.47
1:B:462:PRO:O	1:B:466:TYR:HD2	1.97	0.47
1:A:280:PRO:HA	1:A:281:PRO:HD3	1.85	0.47
1:A:184:ARG:HA	1:A:438:ARG:O	2.14	0.47
1:A:573:LYS:H	1:A:573:LYS:HD3	1.80	0.47
1:B:206:THR:HG23	1:B:210:PHE:HD2	1.79	0.46
1:A:249:ASP:HB2	1:A:251:LYS:HD3	1.97	0.46
1:B:294:LEU:HG	1:B:295:LEU:CD1	2.45	0.46
1:B:573:LYS:H	1:B:573:LYS:HD3	1.81	0.46
1:A:206:THR:HG23	1:A:210:PHE:CD2	2.51	0.46
1:A:226:HIS:CD2	1:A:376:ARG:HA	2.50	0.46
1:B:206:THR:HG23	1:B:210:PHE:CD2	2.51	0.46
1:B:391:MET:HE2	2:B:601:HEM:CMC	2.45	0.46
1:A:251:LYS:HG2	1:A:310:GLN:HG3	1.97	0.46
1:B:249:ASP:HB2	1:B:251:LYS:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:MET:HE2	2:A:601:HEM:CMC	2.46	0.46
1:B:178:SER:HA	1:B:182:LEU:HB2	1.98	0.46
1:A:298:LEU:HD12	1:A:298:LEU:HA	1.72	0.45
1:B:251:LYS:HG2	1:B:310:GLN:HG3	1.97	0.45
1:A:142:PHE:O	1:A:376:ARG:NH2	2.49	0.45
1:A:466:TYR:O	1:A:470:PHE:HD2	1.99	0.45
1:A:461:GLN:C	1:A:462:PRO:O	2.59	0.45
1:B:142:PHE:O	1:B:376:ARG:NH2	2.50	0.45
1:B:573:LYS:HB2	1:B:573:LYS:HE2	1.69	0.45
1:B:270:PRO:O	1:B:272:LEU:N	2.49	0.45
1:B:300:LEU:CD2	1:B:300:LEU:C	2.90	0.45
1:B:408:LEU:HD13	2:B:601:HEM:HBC1	1.99	0.45
1:A:39:TYR:OH	1:A:155:VAL:HG22	2.17	0.45
1:A:178:SER:HA	1:A:182:LEU:HB2	1.98	0.45
1:A:270:PRO:O	1:A:272:LEU:N	2.50	0.45
1:B:226:HIS:CD2	1:B:376:ARG:HA	2.51	0.45
1:B:487:MET:O	1:B:491:LEU:HB2	2.17	0.44
1:A:248:LYS:NZ	1:A:248:LYS:HB3	2.33	0.44
1:A:424:ASP:HB2	1:A:576:PRO:HB2	1.99	0.44
1:B:461:GLN:C	1:B:462:PRO:O	2.59	0.44
1:A:473:LYS:HD3	1:A:473:LYS:N	2.32	0.44
1:B:391:MET:HE2	2:B:601:HEM:HMC2	2.00	0.44
1:B:248:LYS:HB3	1:B:248:LYS:NZ	2.32	0.44
1:B:466:TYR:O	1:B:470:PHE:HD2	1.99	0.44
1:B:473:LYS:HD3	1:B:473:LYS:N	2.32	0.44
1:A:573:LYS:HE2	1:A:573:LYS:HB2	1.68	0.44
1:A:147:TYR:O	1:A:148:TYR:HB2	2.18	0.44
1:A:300:LEU:C	1:A:300:LEU:CD2	2.91	0.44
1:A:424:ASP:O	1:A:428:ARG:HG3	2.17	0.44
1:B:39:TYR:OH	1:B:155:VAL:HG22	2.17	0.44
1:B:298:LEU:HD12	1:B:298:LEU:HA	1.71	0.44
1:A:226:HIS:HD2	1:A:376:ARG:HA	1.83	0.44
1:A:487:MET:O	1:A:491:LEU:HB2	2.18	0.44
1:B:149:THR:O	1:B:378:ALA:HA	2.18	0.43
1:A:554:VAL:O	1:A:558:LEU:HG	2.17	0.43
1:B:147:TYR:O	1:B:148:TYR:HB2	2.19	0.43
1:B:424:ASP:O	1:B:428:ARG:HG3	2.18	0.43
1:B:424:ASP:HB2	1:B:576:PRO:HB2	1.99	0.43
1:B:456:ARG:HA	1:B:456:ARG:CZ	2.49	0.43
1:A:149:THR:O	1:A:378:ALA:HA	2.18	0.43
1:A:481:LEU:CD2	1:A:510:GLU:HA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:PHE:O	1:B:106:THR:HG23	2.18	0.43
1:B:481:LEU:CD2	1:B:510:GLU:HA	2.48	0.43
1:B:554:VAL:O	1:B:558:LEU:HG	2.18	0.43
1:A:478:PHE:O	1:A:481:LEU:HB3	2.19	0.43
1:B:296:PRO:O	1:B:297:GLY:C	2.62	0.43
1:A:408:LEU:HD13	2:A:601:HEM:HBC1	1.99	0.43
1:B:478:PHE:O	1:B:481:LEU:HB3	2.19	0.43
1:A:296:PRO:O	1:A:297:GLY:C	2.62	0.43
1:A:307:ARG:NH2	1:A:419:VAL:HG11	2.34	0.43
1:B:360:LYS:HE2	1:B:362:ASP:HB2	2.01	0.43
1:B:461:GLN:O	1:B:462:PRO:O	2.37	0.43
1:A:102:PHE:O	1:A:106:THR:HG23	2.19	0.42
1:A:456:ARG:CZ	1:A:456:ARG:HA	2.49	0.42
1:A:461:GLN:O	1:A:462:PRO:O	2.37	0.42
1:A:467:ARG:NH1	1:A:472:MET:HB3	2.34	0.42
1:A:391:MET:HE2	2:A:601:HEM:HMC2	2.00	0.42
1:B:307:ARG:NH2	1:B:419:VAL:HG11	2.34	0.42
1:B:190:ASP:HA	1:B:191:PRO:HD2	1.83	0.42
1:B:226:HIS:HD2	1:B:376:ARG:HA	1.85	0.42
1:A:374:ARG:NH2	1:B:374:ARG:HB3	2.35	0.42
1:A:464:ASN:O	1:A:465:GLU:C	2.60	0.42
1:B:150:ARG:HD3	1:B:152:LEU:O	2.19	0.42
1:B:446:HIS:O	1:B:449:VAL:HB	2.20	0.42
1:A:360:LYS:HE2	1:A:362:ASP:HB2	2.01	0.42
1:B:185:ARG:NH2	1:B:438:ARG:HD2	2.30	0.42
1:B:467:ARG:NH1	1:B:472:MET:HB3	2.34	0.42
1:A:454:GLU:O	1:A:458:LEU:HB2	2.20	0.42
1:B:240:ARG:HG3	1:B:271:VAL:CG2	2.49	0.42
1:A:150:ARG:HD3	1:A:152:LEU:O	2.20	0.42
1:A:481:LEU:C	1:A:481:LEU:HD22	2.45	0.42
1:B:464:ASN:O	1:B:465:GLU:C	2.60	0.42
1:B:463:PHE:CE2	1:B:506:GLY:CA	3.03	0.41
1:B:112:LEU:O	1:B:116:VAL:HG23	2.20	0.41
1:B:240:ARG:HH21	1:B:272:LEU:HB3	1.85	0.41
1:B:388:HIS:HB3	1:B:444:ILE:HD12	2.02	0.41
1:B:427:SER:HB3	1:B:577:TYR:CD2	2.55	0.41
1:B:463:PHE:CE2	1:B:507:LEU:N	2.80	0.41
1:B:481:LEU:C	1:B:481:LEU:HD22	2.46	0.41
1:A:74:ILE:HD12	1:A:74:ILE:HA	1.93	0.41
1:A:388:HIS:HB3	1:A:444:ILE:HD12	2.01	0.41
1:A:420:GLU:HG2	1:A:574:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:PHE:CE2	1:A:506:GLY:CA	3.03	0.41
1:B:50:PHE:H	1:B:55:TYR:HA	1.85	0.41
1:B:300:LEU:HD12	1:B:426:PHE:CE2	2.56	0.41
1:A:250:GLY:O	1:A:309:HIS:HE1	2.04	0.41
1:A:456:ARG:HA	1:A:456:ARG:NE	2.35	0.41
1:B:52:LEU:HB3	1:B:53:ASP:H	1.71	0.41
1:B:454:GLU:O	1:B:458:LEU:HB2	2.20	0.41
1:A:142:PHE:HD2	1:B:544:TYR:OH	2.03	0.41
1:A:240:ARG:HG3	1:A:271:VAL:CG2	2.50	0.41
1:A:427:SER:HB3	1:A:577:TYR:CD2	2.56	0.41
1:A:438:ARG:HD2	1:A:438:ARG:HH11	1.73	0.41
1:A:50:PHE:H	1:A:55:TYR:HA	1.86	0.41
1:A:446:HIS:O	1:A:449:VAL:HB	2.20	0.41
1:B:420:GLU:HG3	1:B:572:THR:OG1	2.21	0.41
1:B:280:PRO:HA	1:B:281:PRO:HD3	1.85	0.41
1:A:142:PHE:O	1:A:142:PHE:CE1	2.64	0.40
1:B:456:ARG:HA	1:B:456:ARG:NE	2.35	0.40
1:A:363:PRO:HD2	1:A:545:TRP:CH2	2.56	0.40
1:B:481:LEU:HD12	1:B:501:LEU:CD2	2.51	0.40
1:A:240:ARG:HH21	1:A:272:LEU:HB3	1.86	0.40
1:A:300:LEU:HD12	1:A:426:PHE:CE2	2.56	0.40
1:B:84:PRO:HB2	1:B:88:PHE:HD2	1.86	0.40
1:B:142:PHE:O	1:B:142:PHE:CE1	2.65	0.40
1:B:363:PRO:HD2	1:B:545:TRP:CH2	2.57	0.40
1:A:420:GLU:HG3	1:A:572:THR:OG1	2.22	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	206/554 (37%)	184 (89%)	16 (8%)	6 (3%)	3 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	436/554 (79%)	394 (90%)	33 (8%)	9 (2%)	5	31
All	All	642/1108 (58%)	578 (90%)	49 (8%)	15 (2%)	5	30

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	VAL
1	A	272	LEU
1	B	514	PRO
1	B	584	ASP
1	B	585	PRO
1	B	51	GLY
1	A	52	LEU
1	A	220	PHE
1	A	273	MET
1	B	52	LEU
1	B	220	PHE
1	B	157	ARG
1	A	34	ASN
1	B	520	GLU
1	B	228	VAL

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	489/489 (100%)	413 (84%)	76 (16%)	2	15
1	B	489/489 (100%)	414 (85%)	75 (15%)	3	16
All	All	978/978 (100%)	827 (85%)	151 (15%)	2	16

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ILE

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Mol	Chain	Res	Type
1	A	49	ARG
1	A	52	LEU
1	A	79	ARG
1	A	81	THR
1	A	87	SER
1	A	93	LEU
1	A	97	ARG
1	A	117	LEU
1	A	118	THR
1	A	126	SER
1	A	132	ILE
1	A	140	GLU
1	A	143	SER
1	A	147	TYR
1	A	149	THR
1	A	151	ILE
1	A	154	SER
1	A	163	MET
1	A	165	THR
1	A	169	LYS
1	A	171	LEU
1	A	172	PRO
1	A	182	LEU
1	A	197	MET
1	A	215	LYS
1	A	221	THR
1	A	232	HIS
1	A	239	GLU
1	A	241	GLN
1	A	243	GLN
1	A	261	VAL
1	A	267	GLU
1	A	270	PRO
1	A	271	VAL
1	A	277	ARG
1	A	287	VAL
1	A	289	GLN
1	A	298	LEU
1	A	300	LEU
1	A	310	GLN
1	A	316	LEU
1	A	322	THR

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Mol	Chain	Res	Type
1	A	323	TRP
1	A	341	ILE
1	A	366	LEU
1	A	376	ARG
1	A	377	ILE
1	A	385	TYR
1	A	392	PRO
1	A	399	PRO
1	A	400	GLN
1	A	405	GLU
1	A	411	THR
1	A	412	SER
1	A	433	ARG
1	A	438	ARG
1	A	441	ASP
1	A	467	ARG
1	A	469	ARG
1	A	473	LYS
1	A	481	LEU
1	A	484	GLU
1	A	508	LEU
1	A	514	PRO
1	A	518	PHE
1	A	520	GLU
1	A	530	SER
1	A	534	LEU
1	A	535	LEU
1	A	539	ILE
1	A	545	TRP
1	A	559	VAL
1	A	563	THR
1	A	582	VAL
1	A	586	ARG
1	B	46	ILE
1	B	49	ARG
1	B	52	LEU
1	B	79	ARG
1	B	81	THR
1	B	87	SER
1	B	93	LEU
1	B	97	ARG
1	B	117	LEU

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Mol	Chain	Res	Type
1	B	118	THR
1	B	126	SER
1	B	132	ILE
1	B	140	GLU
1	B	143	SER
1	B	147	TYR
1	B	149	THR
1	B	151	ILE
1	B	154	SER
1	B	163	MET
1	B	165	THR
1	B	169	LYS
1	B	171	LEU
1	B	172	PRO
1	B	182	LEU
1	B	197	MET
1	B	215	LYS
1	B	221	THR
1	B	232	HIS
1	B	239	GLU
1	B	241	GLN
1	B	243	GLN
1	B	261	VAL
1	B	267	GLU
1	B	270	PRO
1	B	271	VAL
1	B	277	ARG
1	B	287	VAL
1	B	289	GLN
1	B	298	LEU
1	B	300	LEU
1	B	310	GLN
1	B	316	LEU
1	B	322	THR
1	B	323	TRP
1	B	341	ILE
1	B	366	LEU
1	B	376	ARG
1	B	377	ILE
1	B	385	TYR
1	B	392	PRO
1	B	399	PRO

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Mol	Chain	Res	Type
1	B	400	GLN
1	B	405	GLU
1	B	411	THR
1	B	412	SER
1	B	433	ARG
1	B	438	ARG
1	B	441	ASP
1	B	467	ARG
1	B	469	ARG
1	B	473	LYS
1	B	481	LEU
1	B	484	GLU
1	B	508	LEU
1	B	514	PRO
1	B	518	PHE
1	B	530	SER
1	B	534	LEU
1	B	535	LEU
1	B	539	ILE
1	B	545	TRP
1	B	559	VAL
1	B	563	THR
1	B	582	VAL
1	B	586	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	56	GLN
1	A	68	ASN
1	A	90	HIS
1	A	203	GLN
1	A	204	HIS
1	A	207	HIS
1	A	208	GLN
1	A	226	HIS
1	A	241	GLN
1	A	309	HIS
1	A	446	HIS
1	B	43	HIS
1	B	68	ASN

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Mol	Chain	Res	Type
1	B	90	HIS
1	B	203	GLN
1	B	204	HIS
1	B	207	HIS
1	B	208	GLN
1	B	226	HIS
1	B	241	GLN
1	B	274	HIS
1	B	309	HIS
1	B	446	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 ⓘ

2 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	$\# Z > 2$
2	HEM	A	601	1	50,50,50	1.34	5 (10%)	67,82,82	1.27	5 (7%)
2	HEM	B	601	1	50,50,50	1.34	5 (10%)	67,82,82	1.28	6 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	601	1	-	7/14/54/54	-
2	HEM	B	601	1	-	7/14/54/54	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEM	CAB-C3B	-3.43	1.38	1.47
2	B	601	HEM	CAC-C3C	-3.38	1.38	1.47
2	A	601	HEM	CAC-C3C	-3.37	1.38	1.47
2	A	601	HEM	CAB-C3B	-3.31	1.38	1.47
2	B	601	HEM	CBB-CAB	3.20	1.45	1.30
2	A	601	HEM	CBB-CAB	3.18	1.45	1.30
2	A	601	HEM	CBC-CAC	2.97	1.44	1.30
2	B	601	HEM	CBC-CAC	2.88	1.44	1.30
2	A	601	HEM	O2A-CGA	-2.24	1.23	1.30
2	B	601	HEM	O2A-CGA	-2.16	1.23	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	CMC-C2C-C1C	3.69	131.23	124.73
2	B	601	HEM	CMC-C2C-C1C	3.57	131.02	124.73
2	A	601	HEM	C3C-C2C-C1C	-2.40	104.77	107.05
2	B	601	HEM	CBD-CAD-C3D	2.24	118.72	112.53
2	B	601	HEM	CAD-CBD-CGD	2.15	119.37	113.67
2	B	601	HEM	C3B-C2B-C1B	-2.13	104.81	106.41
2	A	601	HEM	CAA-C2A-C1A	2.13	129.09	124.94
2	B	601	HEM	C3C-C2C-C1C	-2.11	105.05	107.05
2	A	601	HEM	CAD-CBD-CGD	2.11	119.25	113.67
2	A	601	HEM	CBD-CAD-C3D	2.04	118.19	112.53
2	B	601	HEM	CAA-C2A-C1A	2.04	128.93	124.94

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	HEM	C2B-C3B-CAB-CBB

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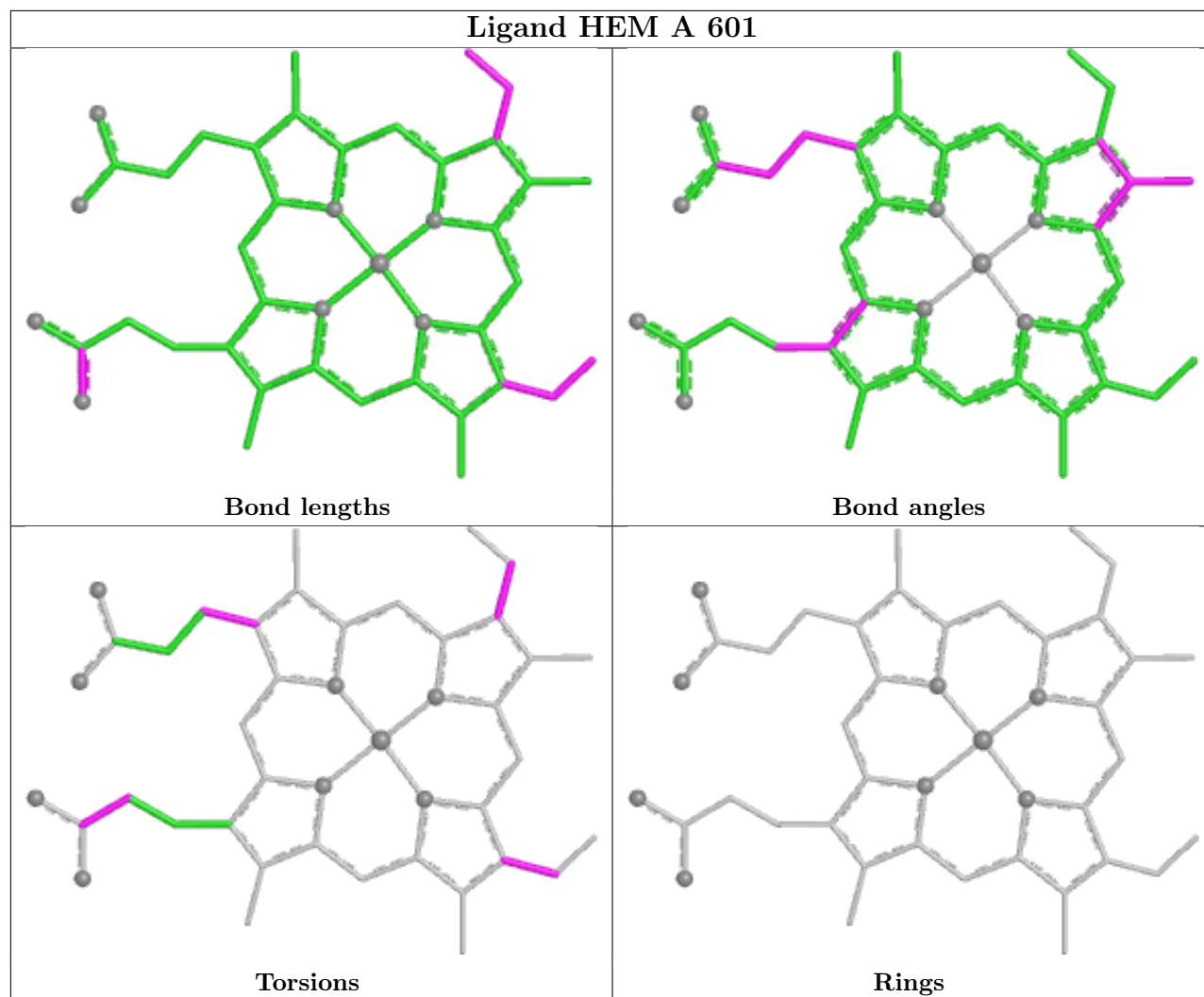
Mol	Chain	Res	Type	Atoms
2	A	601	HEM	C4B-C3B-CAB-CBB
2	A	601	HEM	C2C-C3C-CAC-CBC
2	A	601	HEM	C4C-C3C-CAC-CBC
2	B	601	HEM	C2B-C3B-CAB-CBB
2	B	601	HEM	C4B-C3B-CAB-CBB
2	B	601	HEM	C2C-C3C-CAC-CBC
2	B	601	HEM	C4C-C3C-CAC-CBC
2	A	601	HEM	C4D-C3D-CAD-CBD
2	B	601	HEM	C4D-C3D-CAD-CBD
2	A	601	HEM	CAA-CBA-CGA-O1A
2	B	601	HEM	CAA-CBA-CGA-O1A
2	B	601	HEM	CAA-CBA-CGA-O2A
2	A	601	HEM	CAA-CBA-CGA-O2A

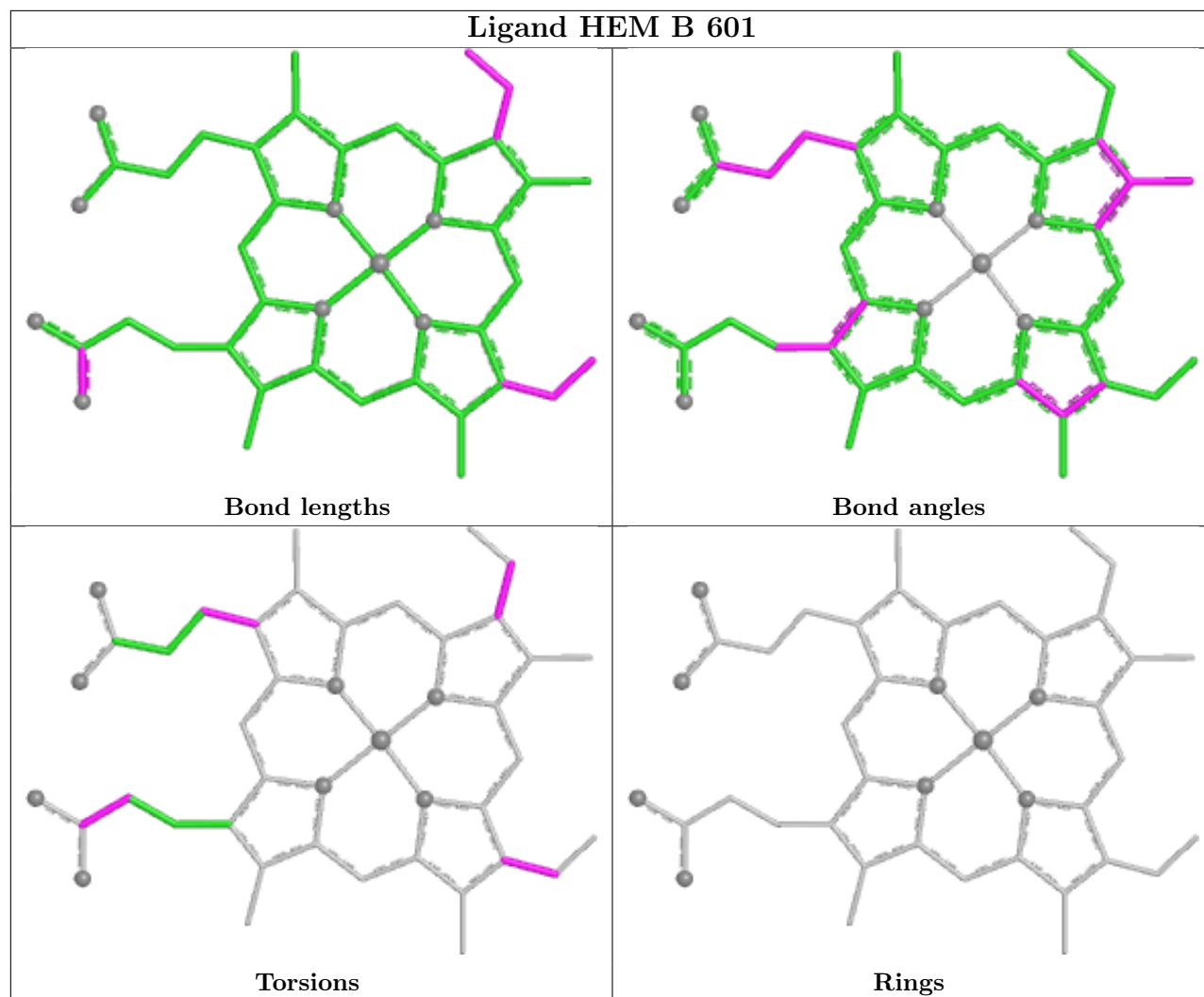
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	4	0
2	B	601	HEM	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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.