



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:35 PM GMT

PDB ID : 1PRH
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

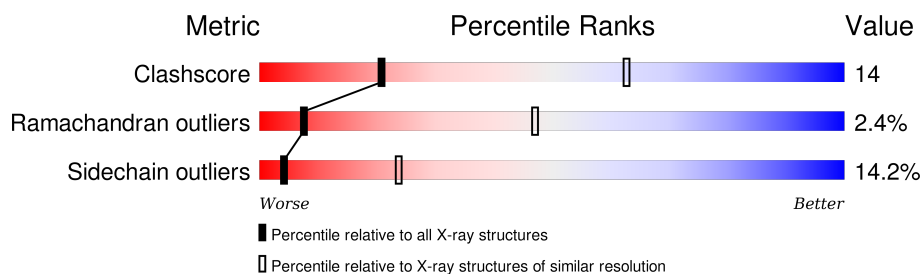
1 Overall quality at a glance

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	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	554	 61% 30% 7% •
1	B	554	 60% 31% 7% •

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9092 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.

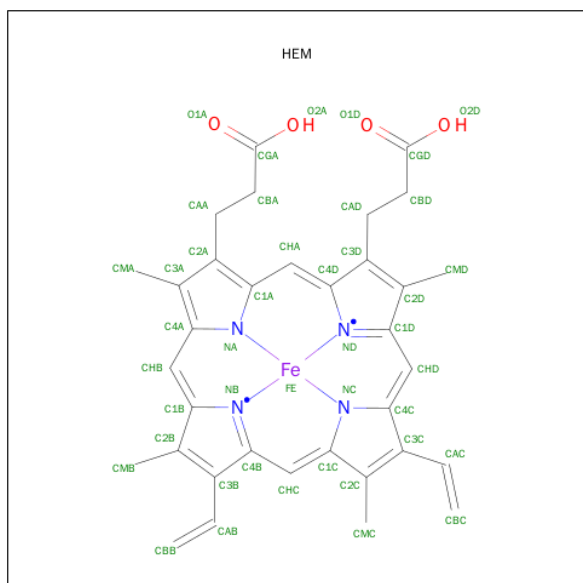
- Molecule 1 is a protein called PROTAGLANDIN H2 SYNTHASE-1.

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

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 (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



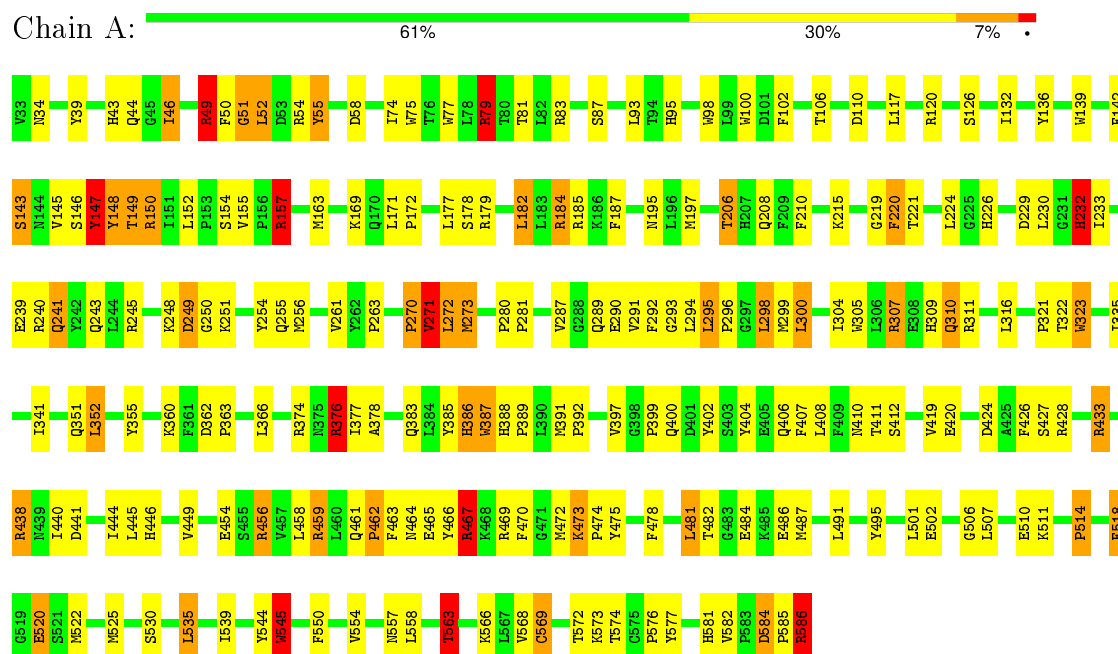
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

3 Residue-property plots

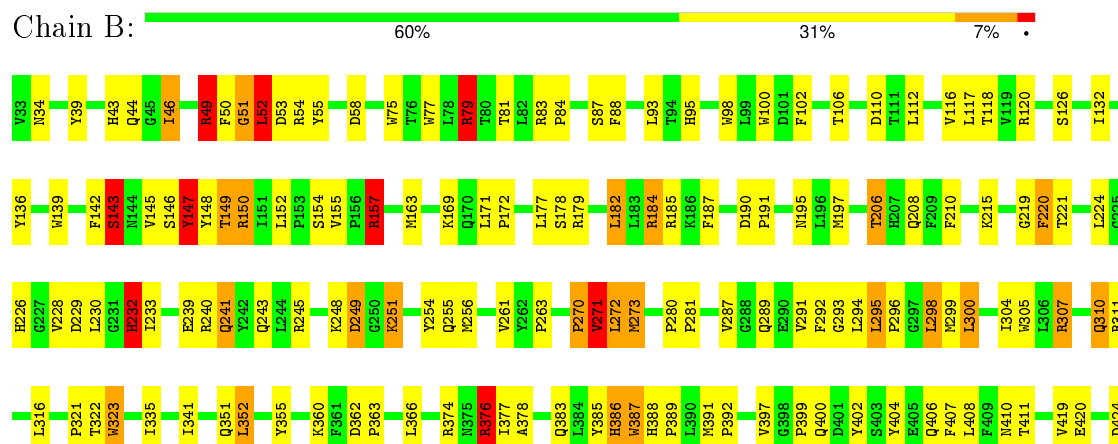
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: PROSTAGLANDIN H2 SYNTHASE-1



• Molecule 1: PROSTAGLANDIN H2 SYNTHASE-1



E510	E511	P514	N515	P518	E519	E520	S521	M522	M525	S530	L535	I539	Y544	M545	F550	V554	M563	K566	L567	C568	T572	K573	P576	Y577	H581	V582	P583	D584	P585	M586	E425	F426	S427	R428	R433	R438	M439	I440	D441	I444	L445	H446	V449	E454	S455	R456	F457	L458	R459	L460	P461	F462	F463	M464	E465	Y466	R467	K468	R469	F470	G471	M472	K473	P474	Y475	F478	L481	T482	G483	E484	K485	E486	M487	L491	Y495	L501	E502	G506	L507
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	99.40 Å 210.30 Å 233.10 Å 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 ⓘ

5.1 Standard geometry ⓘ

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	0.90	2/4642 (0.0%)	1.62	89/6299 (1.4%)
1	B	0.92	2/4642 (0.0%)	1.63	87/6299 (1.4%)
All	All	0.91	4/9284 (0.0%)	1.62	176/12598 (1.4%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	462	PRO	C-N	-5.87	1.20	1.34
1	A	462	PRO	C-N	-5.73	1.20	1.34
1	B	545	TRP	CG-CD2	-5.36	1.34	1.43
1	A	545	TRP	CG-CD2	-5.17	1.34	1.43

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	120	ARG	NE-CZ-NH2	-15.72	112.44	120.30
1	A	143	SER	O-C-N	-15.68	97.61	122.70
1	A	120	ARG	NE-CZ-NH2	-15.54	112.53	120.30
1	B	143	SER	O-C-N	-15.47	97.94	122.70
1	B	120	ARG	NE-CZ-NH1	14.81	127.70	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	ARG	NE-CZ-NH1	14.41	127.50	120.30
1	A	95	HIS	CA-CB-CG	12.47	134.80	113.60
1	B	95	HIS	CA-CB-CG	12.27	134.46	113.60
1	B	49	ARG	NE-CZ-NH1	11.80	126.20	120.30
1	A	49	ARG	NE-CZ-NH1	11.16	125.88	120.30
1	A	143	SER	CA-C-N	10.54	140.38	117.20
1	B	143	SER	CA-C-N	10.39	140.05	117.20
1	A	433	ARG	NE-CZ-NH1	9.99	125.29	120.30
1	B	433	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	A	79	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	B	79	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	B	157	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	A	157	ARG	NE-CZ-NH1	8.81	124.71	120.30
1	A	77	TRP	CD1-CG-CD2	8.57	113.16	106.30
1	B	77	TRP	CD1-CG-CD2	8.43	113.04	106.30
1	B	184	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	A	293	GLY	C-N-CA	8.27	142.38	121.70
1	B	293	GLY	C-N-CA	8.26	142.35	121.70
1	A	184	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	B	569	CYS	CA-CB-SG	-8.01	99.59	114.00
1	B	75	TRP	CE2-CD2-CG	-7.98	100.91	107.30
1	A	569	CYS	CA-CB-SG	-7.98	99.64	114.00
1	A	75	TRP	CE2-CD2-CG	-7.85	101.02	107.30
1	A	305	TRP	CD1-CG-CD2	7.84	112.58	106.30
1	B	544	TYR	CB-CG-CD2	-7.79	116.33	121.00
1	B	467	ARG	NE-CZ-NH2	7.72	124.16	120.30
1	A	100	TRP	CD1-CG-CD2	7.68	112.44	106.30
1	B	323	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	B	100	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	A	305	TRP	CE2-CD2-CG	-7.57	101.24	107.30
1	A	467	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	A	79	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	75	TRP	CD1-CG-CD2	7.44	112.25	106.30
1	A	323	TRP	CE2-CD2-CG	-7.43	101.36	107.30
1	B	305	TRP	CD1-CG-CD2	7.43	112.24	106.30
1	B	75	TRP	CD1-CG-CD2	7.37	112.19	106.30
1	A	544	TYR	CB-CG-CD2	-7.33	116.60	121.00
1	B	376	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	B	387	TRP	CA-CB-CG	7.30	127.58	113.70
1	B	386	HIS	CA-CB-CG	-7.28	101.23	113.60
1	A	386	HIS	CA-CB-CG	-7.25	101.28	113.60
1	B	77	TRP	CE2-CD2-CG	-7.23	101.52	107.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	TRP	CE2-CD2-CG	-7.23	101.52	107.30
1	A	150	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	B	184	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	B	486	GLU	O-C-N	-7.16	111.24	122.70
1	A	387	TRP	CA-CB-CG	7.13	127.25	113.70
1	A	100	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	B	305	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	B	150	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	A	77	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	A	486	GLU	O-C-N	-7.04	111.43	122.70
1	B	387	TRP	CE2-CD2-CG	-6.89	101.78	107.30
1	B	98	TRP	CD1-CG-CD2	6.79	111.73	106.30
1	A	459	ARG	NE-CZ-NH2	6.75	123.67	120.30
1	A	305	TRP	CG-CD2-CE3	6.72	139.95	133.90
1	A	184	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	B	305	TRP	CB-CG-CD1	-6.67	118.33	127.00
1	A	387	TRP	CE2-CD2-CG	-6.66	101.97	107.30
1	B	311	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	A	98	TRP	CD1-CG-CD2	6.65	111.62	106.30
1	B	535	LEU	CA-CB-CG	-6.64	100.02	115.30
1	A	305	TRP	CB-CG-CD1	-6.62	118.39	127.00
1	B	79	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	387	TRP	CD1-CG-CD2	6.62	111.59	106.30
1	B	387	TRP	CD1-CG-CD2	6.58	111.57	106.30
1	B	49	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	98	TRP	CE2-CD2-CG	-6.58	102.04	107.30
1	B	456	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	B	545	TRP	CE2-CD2-CG	-6.51	102.09	107.30
1	A	535	LEU	CA-CB-CG	-6.48	100.40	115.30
1	A	376	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	B	545	TRP	CD1-CG-CD2	6.42	111.44	106.30
1	A	456	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	B	433	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	98	TRP	CE2-CD2-CG	-6.36	102.21	107.30
1	A	433	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	B	219	GLY	N-CA-C	-6.32	97.30	113.10
1	B	586	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	B	586	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	B	305	TRP	CG-CD2-CE3	6.27	139.54	133.90
1	A	311	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	B	545	TRP	CE2-CD2-CE3	6.22	126.17	118.70
1	B	352	LEU	CA-CB-CG	6.22	129.60	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	586	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	B	459	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	B	149	THR	CA-CB-CG2	6.19	121.07	112.40
1	B	83	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	219	GLY	N-CA-C	-6.19	97.64	113.10
1	B	150	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	352	LEU	CA-CB-CG	6.18	129.51	115.30
1	B	299	MET	CG-SD-CE	6.18	110.09	100.20
1	A	149	THR	CA-CB-CG2	6.17	121.04	112.40
1	B	445	LEU	CA-CB-CG	6.17	129.49	115.30
1	A	545	TRP	CE2-CD2-CG	-6.15	102.38	107.30
1	A	100	TRP	CG-CD2-CE3	6.13	139.42	133.90
1	B	323	TRP	NE1-CE2-CD2	6.13	113.43	107.30
1	B	54	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	445	LEU	CA-CB-CG	6.07	129.26	115.30
1	A	49	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	254	TYR	CB-CG-CD2	-6.01	117.39	121.00
1	A	299	MET	CG-SD-CE	6.00	109.79	100.20
1	A	179	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	229	ASP	N-CA-C	-5.97	94.88	111.00
1	A	323	TRP	CD1-CG-CD2	5.96	111.07	106.30
1	A	232	HIS	CA-CB-CG	5.92	123.66	113.60
1	B	232	HIS	CA-CB-CG	5.89	123.61	113.60
1	A	323	TRP	CB-CG-CD1	-5.86	119.39	127.00
1	B	229	ASP	N-CA-C	-5.85	95.22	111.00
1	A	545	TRP	CD1-CG-CD2	5.76	110.91	106.30
1	B	100	TRP	CG-CD2-CE3	5.75	139.07	133.90
1	A	136	TYR	CB-CG-CD1	-5.75	117.55	121.00
1	B	287	VAL	CA-CB-CG2	-5.74	102.30	110.90
1	A	287	VAL	CA-CB-CG2	-5.70	102.35	110.90
1	A	545	TRP	CE2-CD2-CE3	5.70	125.53	118.70
1	A	83	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	323	TRP	NE1-CE2-CD2	5.68	112.98	107.30
1	A	387	TRP	NE1-CE2-CZ2	-5.68	124.16	130.40
1	B	147	TYR	N-CA-C	5.67	126.30	111.00
1	B	387	TRP	CA-C-N	-5.67	104.73	117.20
1	A	586	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	150	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	B	307	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	404	TYR	CB-CG-CD2	-5.61	117.63	121.00
1	A	355	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	A	271	VAL	N-CA-CB	-5.60	99.18	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	355	TYR	CB-CG-CD2	-5.58	117.66	121.00
1	B	323	TRP	CD1-CG-CD2	5.57	110.76	106.30
1	B	323	TRP	NE1-CE2-CZ2	-5.57	124.28	130.40
1	B	271	VAL	N-CA-CB	-5.55	99.28	111.50
1	A	147	TYR	N-CA-C	5.54	125.97	111.00
1	A	387	TRP	CA-C-N	-5.53	105.04	117.20
1	A	456	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	B	387	TRP	NE1-CE2-CZ2	-5.51	124.34	130.40
1	A	307	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	206	THR	N-CA-CB	-5.45	99.94	110.30
1	B	323	TRP	CB-CG-CD1	-5.43	119.94	127.00
1	A	295	LEU	CB-CA-C	-5.43	99.89	110.20
1	B	404	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	A	563	THR	CA-CB-CG2	5.42	119.99	112.40
1	B	291	VAL	CA-CB-CG2	-5.42	102.77	110.90
1	A	291	VAL	CA-CB-CG2	-5.40	102.80	110.90
1	B	545	TRP	NE1-CE2-CD2	5.40	112.70	107.30
1	A	206	THR	N-CA-CB	-5.38	100.08	110.30
1	B	179	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	323	TRP	NE1-CE2-CZ2	-5.37	124.49	130.40
1	B	79	ARG	CD-NE-CZ	5.37	131.12	123.60
1	B	295	LEU	CB-CA-C	-5.37	100.00	110.20
1	B	307	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	B	525	MET	CG-SD-CE	-5.34	91.66	100.20
1	A	77	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	B	387	TRP	CG-CD2-CE3	5.29	138.66	133.90
1	A	525	MET	CG-SD-CE	-5.28	91.75	100.20
1	A	545	TRP	NE1-CE2-CD2	5.27	112.57	107.30
1	B	136	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	B	254	TYR	CB-CG-CD2	-5.24	117.85	121.00
1	A	54	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	B	563	THR	CA-CB-CG2	5.21	119.69	112.40
1	A	387	TRP	CG-CD2-CE3	5.16	138.54	133.90
1	A	323	TRP	CG-CD2-CE3	5.16	138.54	133.90
1	B	323	TRP	CG-CD2-CE3	5.13	138.52	133.90
1	A	229	ASP	CA-C-N	5.13	128.49	117.20
1	A	293	GLY	O-C-N	-5.11	114.52	122.70
1	A	149	THR	CA-CB-OG1	-5.11	98.27	109.00
1	B	287	VAL	CA-CB-CG1	5.09	118.53	110.90
1	A	77	TRP	CB-CG-CD1	-5.08	120.40	127.00
1	A	147	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	B	229	ASP	CA-C-N	5.07	128.36	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ARG	CD-NE-CZ	5.05	130.67	123.60
1	B	157	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	B	251	LYS	CA-C-N	-5.03	106.14	117.20

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	4410	131	0
1	B	4503	0	4410	132	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
All	All	9092	0	8880	259	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 14.

All (259) 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:CD1	1:A:142:PHE:O	1.98	1.15
1:B:142:PHE:O	1:B:142:PHE:CD1	1.98	1.15
1:B:462:PRO:HG2	1:B:465:GLU:HG2	1.36	1.06
1:A:142:PHE:CD1	1:A:142:PHE:C	2.30	1.05
1:B:142:PHE:C	1:B:142:PHE:CD1	2.30	1.03
1:A:462:PRO:HG2	1:A:465:GLU:HG2	1.36	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:461:GLN:HB3	1:B:462:PRO:HD2	1.60	0.82
1:A:461:GLN:HB3	1:A:462:PRO:HD2	1.59	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:482:THR:O	1:A:511:LYS:HB3	1.89	0.72
1:B:142:PHE:C	1:B:142:PHE:HD1	1.92	0.72
1:A:464:ASN:HA	1:A:467:ARG:HB2	1.72	0.72
1:A:142:PHE:HD1	1:A:142:PHE:C	1.93	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:HE2	1:B:506:GLY:C	1.95	0.70
1:A:185:ARG:HH21	1:A:438:ARG:HD2	1.57	0.70
1:A:463:PHE:HE2	1:A:506:GLY:C	1.95	0.69
1:B:463:PHE:HE2	1:B:507:LEU:N	1.89	0.69
1:A:463:PHE:HE2	1:A:507:LEU:N	1.89	0.69
1:B:185:ARG:HH21	1:B:438:ARG:HD2	1.56	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:B:463:PHE:CE2	1:B:506:GLY:C	2.70	0.65
1:A:157:ARG:HA	1:A:459:ARG:NH1	2.12	0.65
1:A:463:PHE:CE2	1:A:506:GLY:C	2.70	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:195:ASN:HB3	1:A:582:VAL:HG23	1.84	0.60
1:A:145:VAL:HG13	1:A:224:LEU:HD23	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:B:461:GLN:CB	1:B:462:PRO:HD2	2.31	0.56
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:A:461:GLN:CB	1:A:462:PRO:HD2	2.31	0.56
1:B:49:ARG:HH11	1:B:49:ARG:HG3	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:461:GLN:HB3	1:B:462:PRO:CD	2.31	0.55
1:B:241:GLN:HE22	1:B:245:ARG:HH11	1.54	0.55
1:A:241:GLN:HE22	1:A:245:ARG:HH11	1.54	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:A:389:PRO:HG3	1:A:440:ILE:HG12	1.89	0.54
1:B:46:ILE:HG23	1:B:58:ASP:HB3	1.89	0.54
1:A:586:ARG:NE	1:A:586:ARG:HA	2.22	0.54
1:A:46:ILE:HG23	1:A:58:ASP:HB3	1.90	0.53
1:B:464:ASN:OD1	1:B:474:PRO:HA	2.08	0.53
1:B:586:ARG:NE	1:B:586:ARG:HA	2.23	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
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:HE	1:A:586:ARG:HA	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:TYR:OH	1:B:502:GLU:HG3	2.09	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:A:383:GLN:O	1:A:386:HIS:HB2	2.10	0.52
1:B:473:LYS:HD3	1:B:473:LYS:H	1.74	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:A:232:HIS:CD2	1:A:233:ILE:HG13	2.45	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:142:PHE:CG	1:A:142:PHE:O	2.60	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:B:462:PRO:CG	1:B:465:GLU:HG2	2.26	0.50
1:A:461:GLN:CB	1:A:462:PRO:CD	2.89	0.50
1:B:464:ASN:HD21	1:B:475:TYR:N	2.09	0.50
1:A:79:ARG:HH11	1:A:79:ARG:HG2	1.77	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: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:461:GLN:CB	1:B:462:PRO:CD	2.89	0.49
1:B:463:PHE:CE2	1:B:506:GLY:HA3	2.47	0.49
1:A:185:ARG:NH2	1:A:438:ARG:HH11	2.11	0.49
1:A:208:GLN:HB3	1:A:232:HIS:ND1	2.28	0.49
1:B:467:ARG:HH12	1:B:473:LYS:NZ	2.11	0.49
1:A:406:GLN:O	1:A:410:ASN:HB2	2.12	0.49
1:A:481:LEU:CD2	1:A:481:LEU:C	2.81	0.49
1:B:185:ARG:NH2	1:B:438:ARG:HH11	2.10	0.49
1:B:79:ARG:HH11	1:B:79:ARG:HG2	1.78	0.49
1:A:43:HIS:O	1:A:44:GLN:HG2	2.13	0.49
1:B:241:GLN:HE21	1:B:245:ARG:HD2	1.78	0.49
1:A:467:ARG:HH12	1:A:473:LYS:NZ	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLN:HG2	1:A:263:PRO:O	2.13	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:481:LEU:CD2	1:B:481:LEU:C	2.81	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:B:481:LEU:HD12	1:B:501:LEU:HD22	1.96	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: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:B:462:PRO:O	1:B:466:TYR:HD2	1.97	0.47
1:A:294:LEU:HG	1:A:295:LEU:CD1	2.45	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:B:294:LEU:HG	1:B:295:LEU:CD1	2.45	0.46
1:B:573:LYS:HD3	1:B:573:LYS:H	1.81	0.46
1:A:249:ASP:HB2	1:A:251:LYS:HD3	1.97	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: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
1:B:178:SER:HA	1:B:182:LEU:HB2	1.98	0.46
1:A:298:LEU:HA	1:A:298:LEU:HD12	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: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:408:LEU:HD13	2:B:601:HEM:HBC1	1.99	0.45
1:B:270:PRO:O	1:B:272:LEU:N	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:HIS:CD2	1:B:376:ARG:HA	2.51	0.45
1:A:270:PRO:O	1:A:272:LEU:N	2.50	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:B:487:MET:O	1:B:491:LEU:HB2	2.17	0.44
1:A:248:LYS:HB3	1:A:248:LYS:NZ	2.33	0.44
1:A:424:ASP:HB2	1:A:576:PRO:HB2	1.99	0.44
1:A:473:LYS:N	1:A:473:LYS:HD3	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:B:248:LYS:NZ	1:B:248:LYS:HB3	2.32	0.44
1:A:573:LYS:HB2	1:A:573:LYS:HE2	1.68	0.44
1:A:147:TYR:O	1:A:148:TYR:HB2	2.18	0.44
1:B:298:LEU:HD12	1:B:298:LEU:HA	1.71	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: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:B:147:TYR:O	1:B:148:TYR:HB2	2.19	0.43
1:A:554:VAL:O	1:A:558:LEU:HG	2.17	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:B:481:LEU:CD2	1:B:510:GLU:HA	2.48	0.43
1:A:481:LEU:CD2	1:A:510:GLU:HA	2.49	0.43
1:B:102:PHE:O	1:B:106:THR:HG23	2.18	0.43
1:A:149:THR:O	1:A:378:ALA:HA	2.18	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:478:PHE:O	1:B:481:LEU:HB3	2.19	0.43
1:A:408:LEU:HD13	2:A:601:HEM:HBC1	1.99	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:456:ARG:CZ	1:A:456:ARG:HA	2.49	0.42
1:A:102:PHE:O	1:A:106:THR:HG23	2.19	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:B:307:ARG:NH2	1:B:419:VAL:HG11	2.34	0.42
1:B:226:HIS:HD2	1:B:376:ARG:HA	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ASP:HA	1:B:191:PRO:HD2	1.83	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:374:ARG:NH2	1:B:374:ARG:HB3	2.35	0.42
1:B:467:ARG:NH1	1:B:472:MET:HB3	2.34	0.42
1:B:185:ARG:NH2	1:B:438:ARG:HD2	2.30	0.42
1:A:360:LYS:HE2	1:A:362:ASP:HB2	2.01	0.42
1:B:240:ARG:HG3	1:B:271:VAL:CG2	2.49	0.42
1:A:454:GLU:O	1:A:458:LEU:HB2	2.20	0.42
1:A:150:ARG:HD3	1:A:152:LEU:O	2.20	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:463:PHE:CE2	1:B:507:LEU:N	2.80	0.41
1:B:240:ARG:HH21	1:B:272:LEU:HB3	1.85	0.41
1:B:427:SER:HB3	1:B:577:TYR:CD2	2.55	0.41
1:B:388:HIS:HB3	1:B:444:ILE:HD12	2.02	0.41
1:A:240:ARG:HH22	1:A:273:MET:HE2	1.85	0.41
1:A:74:ILE:HD12	1:A:74:ILE:HA	1.93	0.41
1:A:463:PHE:CE2	1:A:506:GLY:CA	3.03	0.41
1:A:420:GLU:HG2	1:A:574:THR:HG22	2.03	0.41
1:A:388:HIS:HB3	1:A:444:ILE:HD12	2.01	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:456:ARG:NE	1:A:456:ARG:HA	2.35	0.41
1:B:52:LEU:HB3	1:B:53:ASP:H	1.71	0.41
1:A:250:GLY:O	1:A:309:HIS:HE1	2.04	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:438:ARG:HH11	1:A:438:ARG:HD2	1.73	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:B:420:GLU:HG3	1:B:572:THR:OG1	2.21	0.41
1:B:240:ARG:HH22	1:B:273:MET:HE2	1.84	0.41
1:A:446:HIS:O	1:A:449:VAL:HB	2.20	0.41
1:A:50:PHE:H	1:A:55:TYR:HA	1.86	0.41
1:B:280:PRO:HA	1:B:281:PRO:HD3	1.85	0.41
1:A:142:PHE:CE1	1:A:142:PHE:O	2.64	0.40
1:B:456:ARG:HA	1:B:456:ARG:NE	2.35	0.40
1:B:481:LEU:HD12	1:B:501:LEU:CD2	2.51	0.40
1:A:273:MET:HE2	1:A:290:GLU:HA	2.03	0.40
1:A:363:PRO:HD2	1:A:545:TRP:CH2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:PHE:O	1:B:142:PHE:CE1	2.65	0.40
1:A:461:GLN:C	1:A:462:PRO:O	2.59	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: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 [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	552/554 (100%)	493 (89%)	46 (8%)	13 (2%)	7	47
1	B	552/554 (100%)	493 (89%)	46 (8%)	13 (2%)	7	47
All	All	1104/1108 (100%)	986 (89%)	92 (8%)	26 (2%)	7	47

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	VAL
1	A	272	LEU
1	A	514	PRO
1	A	584	ASP
1	A	585	PRO
1	B	271	VAL
1	B	272	LEU
1	B	514	PRO
1	B	584	ASP
1	B	585	PRO
1	A	51	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	273	MET
1	A	157	ARG
1	B	157	ARG
1	A	34	ASN
1	A	520	GLU
1	B	34	ASN
1	B	520	GLU
1	A	148	TYR
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%)	420 (86%)	69 (14%)	4	24
1	B	489/489 (100%)	419 (86%)	70 (14%)	4	24
All	All	978/978 (100%)	839 (86%)	139 (14%)	4	24

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	49	ARG
1	A	52	LEU
1	A	55	TYR
1	A	79	ARG
1	A	81	THR
1	A	87	SER
1	A	93	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	110	ASP
1	A	117	LEU
1	A	126	SER
1	A	132	ILE
1	A	147	TYR
1	A	154	SER
1	A	163	MET
1	A	169	LYS
1	A	171	LEU
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	249	ASP
1	A	256	MET
1	A	261	VAL
1	A	270	PRO
1	A	271	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
1	A	323	TRP
1	A	341	ILE
1	A	351	GLN
1	A	352	LEU
1	A	366	LEU
1	A	376	ARG
1	A	377	ILE
1	A	385	TYR
1	A	387	TRP
1	A	392	PRO
1	A	399	PRO
1	A	400	GLN
1	A	411	THR
1	A	412	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	514	PRO
1	A	518	PHE
1	A	520	GLU
1	A	530	SER
1	A	535	LEU
1	A	539	ILE
1	A	545	TRP
1	A	557	ASN
1	A	563	THR
1	A	581	HIS
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	110	ASP
1	B	117	LEU
1	B	118	THR
1	B	126	SER
1	B	132	ILE
1	B	143	SER
1	B	147	TYR
1	B	154	SER
1	B	163	MET
1	B	169	LYS
1	B	171	LEU
1	B	182	LEU
1	B	197	MET
1	B	215	LYS
1	B	221	THR
1	B	232	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	239	GLU
1	B	241	GLN
1	B	243	GLN
1	B	249	ASP
1	B	256	MET
1	B	261	VAL
1	B	270	PRO
1	B	271	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	351	GLN
1	B	352	LEU
1	B	366	LEU
1	B	376	ARG
1	B	377	ILE
1	B	385	TYR
1	B	387	TRP
1	B	392	PRO
1	B	399	PRO
1	B	400	GLN
1	B	411	THR
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	514	PRO
1	B	515	ASN
1	B	518	PHE
1	B	530	SER
1	B	535	LEU
1	B	539	ILE
1	B	545	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	557	ASN
1	B	563	THR
1	B	573	LYS
1	B	581	HIS
1	B	586	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	68	ASN
1	A	204	HIS
1	A	207	HIS
1	A	208	GLN
1	A	226	HIS
1	A	241	GLN
1	A	243	GLN
1	A	309	HIS
1	A	443	HIS
1	B	56	GLN
1	B	68	ASN
1	B	204	HIS
1	B	207	HIS
1	B	208	GLN
1	B	226	HIS
1	B	241	GLN
1	B	243	GLN
1	B	309	HIS
1	B	443	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 carbohydrates 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	30,50,50	2.95	10 (33%)	24,82,82	2.10	8 (33%)
2	HEM	B	601	1	30,50,50	2.92	9 (30%)	24,82,82	2.08	8 (33%)

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	-	0/10/54/54	0/0/8/8
2	HEM	B	601	1	-	0/10/54/54	0/0/8/8

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C3B-C4B	-7.71	1.45	1.51
2	B	601	HEM	C3B-CAB	-6.97	1.38	1.51
2	B	601	HEM	C3C-CAC	-6.91	1.38	1.51
2	A	601	HEM	C3C-CAC	-6.90	1.38	1.51
2	B	601	HEM	C3B-C4B	-6.87	1.45	1.51
2	A	601	HEM	C3B-CAB	-6.81	1.38	1.51
2	A	601	HEM	C2D-C3D	-6.68	1.34	1.54
2	B	601	HEM	C2D-C3D	-6.38	1.35	1.54
2	B	601	HEM	C3D-C4D	-5.17	1.44	1.51
2	A	601	HEM	C3D-C4D	-4.51	1.45	1.51
2	B	601	HEM	C2C-C1C	-2.69	1.47	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C2C-C1C	-2.49	1.47	1.52
2	A	601	HEM	C2B-C1B	-2.08	1.45	1.51
2	B	601	HEM	C1C-NC	2.31	1.38	1.36
2	A	601	HEM	C1C-NC	2.33	1.38	1.36
2	B	601	HEM	CBC-CAC	2.58	1.44	1.29
2	A	601	HEM	CBC-CAC	2.65	1.44	1.29
2	A	601	HEM	CBB-CAB	2.83	1.45	1.29
2	B	601	HEM	CBB-CAB	2.84	1.45	1.29

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	C3C-CAC-CBC	-2.09	121.25	124.46
2	B	601	HEM	C3C-CAC-CBC	-2.06	121.29	124.46
2	B	601	HEM	CBA-CAA-C2A	2.15	116.39	112.53
2	A	601	HEM	CBA-CAA-C2A	2.22	116.50	112.53
2	B	601	HEM	CMD-C2D-C3D	2.63	125.98	114.35
2	A	601	HEM	CMD-C2D-C3D	2.67	126.14	114.35
2	B	601	HEM	C2D-C3D-C4D	2.77	106.19	101.50
2	A	601	HEM	C2D-C3D-C4D	2.78	106.21	101.50
2	B	601	HEM	CMC-C2C-C3C	2.96	123.91	116.53
2	A	601	HEM	CMC-C2C-C3C	2.98	123.98	116.53
2	A	601	HEM	CAD-C3D-C4D	4.17	127.19	112.47
2	B	601	HEM	CAD-C3D-C2D	4.18	125.23	113.22
2	B	601	HEM	CMB-C2B-C3B	4.26	127.17	116.53
2	A	601	HEM	CAD-C3D-C2D	4.31	125.61	113.22
2	B	601	HEM	CAD-C3D-C4D	4.31	127.68	112.47
2	A	601	HEM	CMB-C2B-C3B	4.32	127.31	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.