



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:09 PM UTC

PDB ID : 3CP4 / pdb_00003cp4
Title : CRYSTAL STRUCTURE OF THE CYTOCHROME P450-CAM ACTIVE
SITE MUTANT THR252ALA
Authors : Raag, R.; Poulos, T.L.
Deposited on : 1991-06-04
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

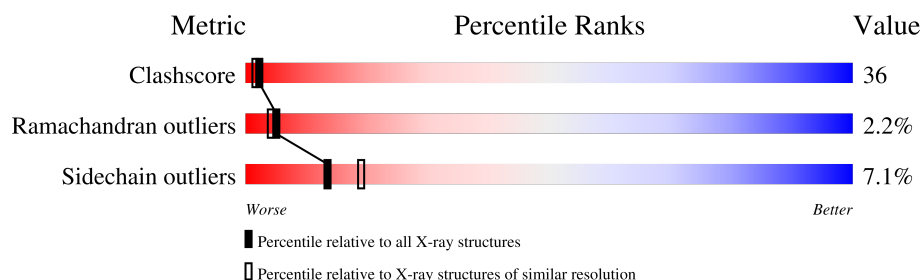
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	414	28% 43% 23% • •

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	ADM	A	416	-	-	X	-

2 Entry composition [i](#)

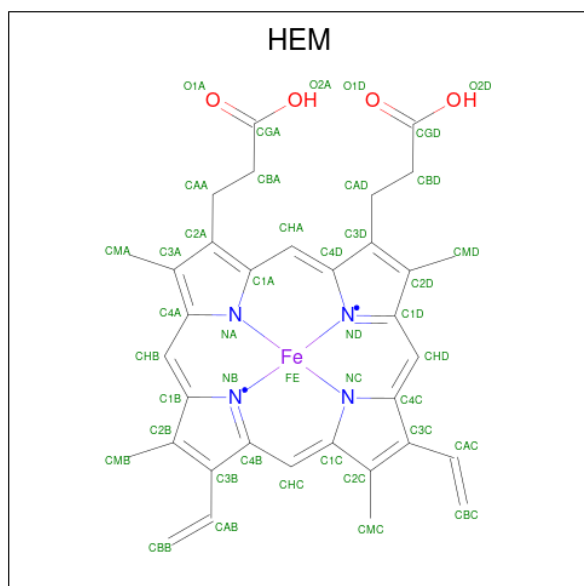
There are 4 unique types of molecules in this entry. The entry contains 3465 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CYTOCHROME P450-CAM.

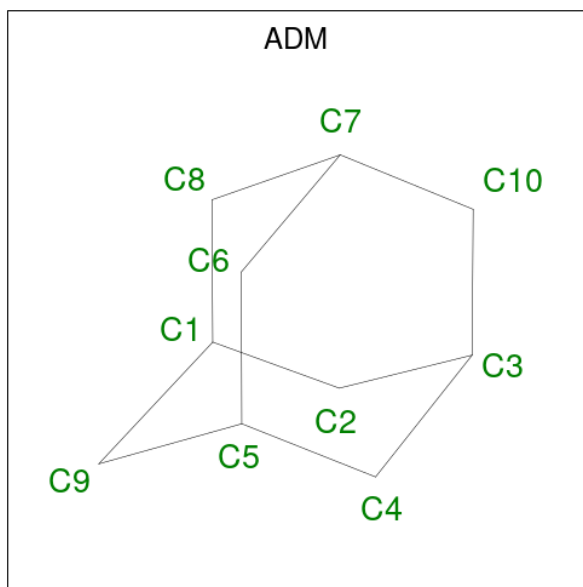
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3208	2033	560	597	18			

- 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		

- Molecule 3 is ADAMANTANE (CCD ID: ADM) (formula: $C_{10}H_{16}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 10 10	0	0

- Molecule 4 is water.

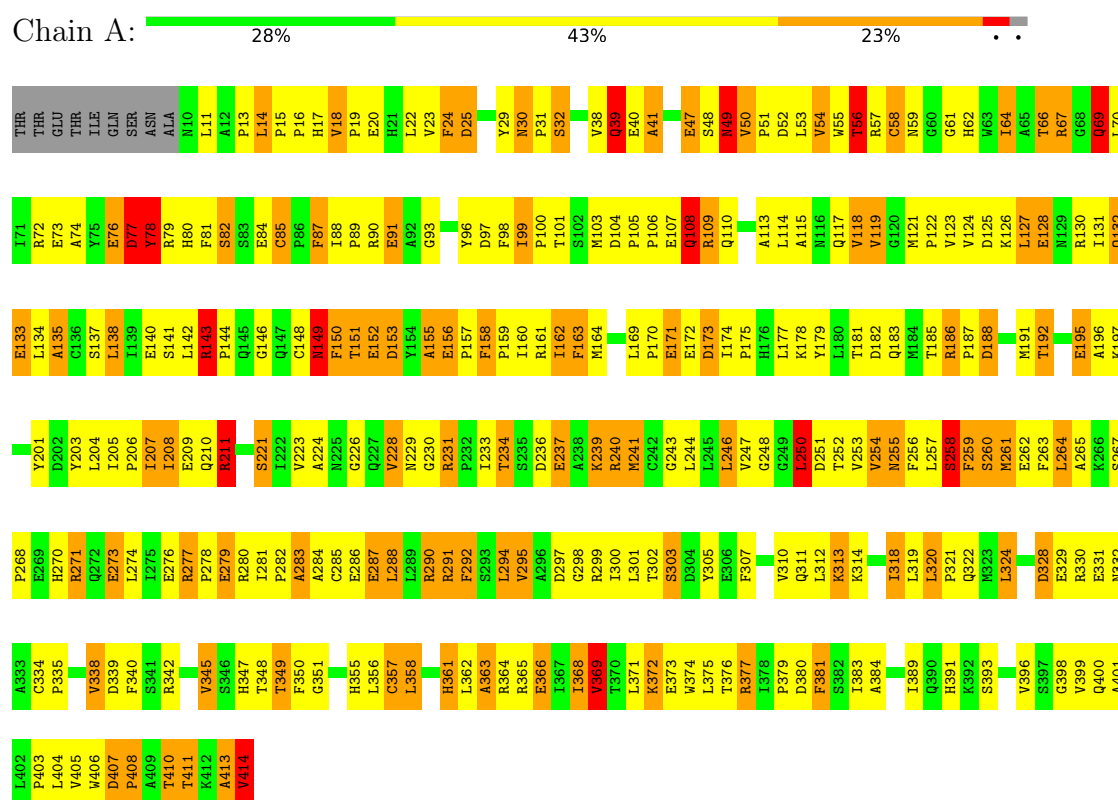
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	204	Total O 204 204	0	0

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: CYTOCHROME P450-CAM



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.67Å 103.90Å 36.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.163 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3465	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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: ADM, 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	1.49	8/3287 (0.2%)	2.47	224/4465 (5.0%)

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	10

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	LEU	N-CA	6.33	1.54	1.46
1	A	257	LEU	C-N	-6.20	1.26	1.33
1	A	66	THR	CA-CB	6.19	1.64	1.53
1	A	324	LEU	C-N	-6.08	1.26	1.33
1	A	294	LEU	C-O	5.79	1.30	1.23
1	A	276	GLU	CD-OE1	5.45	1.35	1.25
1	A	64	ILE	C-N	-5.24	1.26	1.33
1	A	77	ASP	C-O	5.23	1.30	1.24

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	PHE	CA-CB-CG	12.43	126.23	113.80
1	A	211	ARG	CD-NE-CZ	11.46	140.45	124.40
1	A	118	VAL	N-CA-C	11.30	121.16	110.53
1	A	324	LEU	N-CA-C	11.22	124.61	111.71
1	A	357	CYS	CA-C-N	10.93	135.82	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	CYS	C-N-CA	10.93	135.82	120.29
1	A	366	GLU	CB-CG-CD	10.90	131.14	112.60
1	A	195	GLU	CA-CB-CG	10.86	135.82	114.10
1	A	133	GLU	CB-CG-CD	10.27	130.06	112.60
1	A	209	GLU	CA-CB-CG	10.18	134.46	114.10
1	A	223	VAL	CB-CA-C	10.08	125.23	112.02
1	A	183	GLN	OE1-CD-NE2	-9.68	112.92	122.60
1	A	52	ASP	CA-CB-CG	9.52	122.12	112.60
1	A	132	GLN	CA-CB-CG	9.21	132.51	114.10
1	A	149	ASN	CA-C-O	-9.20	110.02	121.89
1	A	47	GLU	CA-C-N	8.96	132.66	120.38
1	A	47	GLU	C-N-CA	8.96	132.66	120.38
1	A	398	GLY	N-CA-C	8.93	126.19	111.27
1	A	259	PHE	CA-CB-CG	8.81	122.61	113.80
1	A	195	GLU	CB-CG-CD	8.67	127.34	112.60
1	A	407	ASP	CA-C-O	8.44	126.45	119.36
1	A	403	PRO	CA-C-O	-8.41	111.08	120.92
1	A	405	VAL	CA-C-O	-8.40	111.52	120.76
1	A	138	LEU	CA-CB-CG	8.39	145.65	116.30
1	A	251	ASP	CB-CA-C	7.99	121.72	109.34
1	A	66	THR	N-CA-C	7.97	123.22	113.17
1	A	156	GLU	CB-CG-CD	7.91	126.05	112.60
1	A	186	ARG	CD-NE-CZ	7.85	135.39	124.40
1	A	248	GLY	N-CA-C	-7.79	103.03	113.24
1	A	260	SER	N-CA-CB	7.75	121.52	110.12
1	A	374	TRP	CB-CA-C	7.61	123.79	110.85
1	A	84	GLU	CA-CB-CG	7.50	129.09	114.10
1	A	108	GLN	CA-CB-CG	7.48	129.05	114.10
1	A	58	CYS	CB-CA-C	7.47	122.12	109.50
1	A	90	ARG	CD-NE-CZ	7.47	134.86	124.40
1	A	130	ARG	CD-NE-CZ	7.42	134.78	124.40
1	A	152	GLU	N-CA-CB	7.39	121.74	110.28
1	A	210	GLN	CA-CB-CG	7.34	128.79	114.10
1	A	158	PHE	CA-CB-CG	7.33	121.13	113.80
1	A	251	ASP	N-CA-C	7.32	122.77	113.55
1	A	369	VAL	CA-CB-CG1	7.29	122.80	110.40
1	A	118	VAL	CA-C-N	7.27	132.24	121.77
1	A	118	VAL	C-N-CA	7.27	132.24	121.77
1	A	38	VAL	CA-C-O	-7.27	112.98	121.05
1	A	287	GLU	CA-CB-CG	7.21	128.52	114.10
1	A	104	ASP	CB-CA-C	7.20	120.82	109.37
1	A	101	THR	N-CA-CB	7.17	120.38	109.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	LYS	N-CA-CB	7.14	120.62	110.12
1	A	254	VAL	N-CA-CB	-7.13	103.13	110.62
1	A	152	GLU	CA-CB-CG	7.05	128.19	114.10
1	A	69	GLN	CA-C-O	-7.02	112.98	120.42
1	A	64	ILE	CA-C-O	-6.89	112.17	120.78
1	A	345	VAL	N-CA-CB	6.84	119.72	111.31
1	A	18	VAL	O-C-N	6.79	127.48	121.57
1	A	39	GLN	N-CA-CB	6.79	120.10	110.12
1	A	179	TYR	N-CA-C	-6.78	103.89	111.28
1	A	209	GLU	CB-CG-CD	6.78	124.12	112.60
1	A	110	GLN	CB-CG-CD	6.76	124.10	112.60
1	A	130	ARG	N-CA-CB	6.67	120.61	110.28
1	A	66	THR	OG1-CB-CG2	6.64	122.57	109.30
1	A	383	ILE	N-CA-CB	6.58	118.40	110.31
1	A	328	ASP	CA-CB-CG	6.57	119.17	112.60
1	A	50	VAL	CB-CA-C	6.56	117.39	110.37
1	A	209	GLU	CA-C-N	6.56	129.95	120.38
1	A	209	GLU	C-N-CA	6.56	129.95	120.38
1	A	410	THR	CA-CB-OG1	-6.54	99.79	109.60
1	A	307	PHE	CA-CB-CG	6.53	120.33	113.80
1	A	47	GLU	CA-CB-CG	6.48	127.06	114.10
1	A	124	VAL	CA-C-O	-6.48	114.31	121.17
1	A	221	SER	N-CA-CB	6.46	119.72	110.16
1	A	228	VAL	N-CA-C	6.46	118.10	106.61
1	A	135	ALA	N-CA-C	-6.44	104.18	111.07
1	A	78	TYR	N-CA-C	6.44	120.71	112.34
1	A	338	VAL	N-CA-CB	-6.42	103.75	110.95
1	A	292	PHE	CB-CA-C	6.36	119.98	111.14
1	A	259	PHE	N-CA-C	-6.35	104.28	111.14
1	A	137	SER	CA-C-O	-6.35	113.78	120.63
1	A	237	GLU	CB-CG-CD	6.33	123.35	112.60
1	A	288	LEU	CA-CB-CG	6.32	138.41	116.30
1	A	126	LYS	CA-C-O	-6.32	114.14	120.90
1	A	132	GLN	OE1-CD-NE2	-6.24	116.36	122.60
1	A	64	ILE	O-C-N	6.22	130.35	122.57
1	A	295	VAL	CB-CA-C	6.22	120.94	111.68
1	A	262	GLU	CB-CG-CD	6.21	123.16	112.60
1	A	413	ALA	N-CA-C	-6.20	102.18	110.55
1	A	158	PHE	N-CA-CB	6.20	121.40	110.37
1	A	253	VAL	N-CA-CB	6.17	118.93	110.54
1	A	311	GLN	OE1-CD-NE2	-6.17	116.43	122.60
1	A	330	ARG	NE-CZ-NH2	6.17	124.75	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	PHE	CA-CB-CG	-6.16	107.64	113.80
1	A	363	ALA	O-C-N	6.15	129.16	122.15
1	A	403	PRO	O-C-N	6.14	129.54	123.03
1	A	153	ASP	N-CA-C	6.13	118.93	111.82
1	A	287	GLU	CA-C-O	-6.12	114.06	120.55
1	A	285	CYS	O-C-N	6.10	129.10	122.15
1	A	279	GLU	CA-CB-CG	6.08	126.26	114.10
1	A	329	GLU	CB-CG-CD	6.04	122.87	112.60
1	A	78	TYR	CA-C-N	6.04	133.07	121.54
1	A	78	TYR	C-N-CA	6.04	133.07	121.54
1	A	294	LEU	CA-C-O	-6.04	111.88	118.52
1	A	405	VAL	O-C-N	6.01	129.72	123.05
1	A	32	SER	N-CA-C	6.00	117.51	110.97
1	A	127	LEU	N-CA-C	6.00	120.44	113.18
1	A	110	GLN	CA-CB-CG	6.00	126.09	114.10
1	A	40	GLU	CA-CB-CG	6.00	126.09	114.10
1	A	76	GLU	CB-CG-CD	5.99	122.79	112.60
1	A	371	LEU	CB-CA-C	5.99	120.36	110.90
1	A	311	GLN	N-CA-CB	5.96	119.48	109.94
1	A	40	GLU	N-CA-CB	5.96	119.40	110.22
1	A	188	ASP	O-C-N	5.96	129.17	122.32
1	A	124	VAL	CB-CA-C	5.95	119.58	111.97
1	A	155	ALA	CA-C-O	-5.95	114.76	121.00
1	A	264	LEU	CB-CA-C	5.94	120.95	110.85
1	A	113	ALA	N-CA-CB	5.94	119.36	110.22
1	A	241	MET	N-CA-CB	5.92	118.65	110.07
1	A	365	ARG	CA-C-O	-5.91	113.42	120.10
1	A	66	THR	CA-CB-OG1	-5.90	100.75	109.60
1	A	48	SER	O-C-N	5.88	128.35	122.12
1	A	115	ALA	CB-CA-C	5.88	120.54	110.79
1	A	133	GLU	CB-CA-C	-5.84	100.75	110.68
1	A	365	ARG	NE-CZ-NH1	5.84	127.34	121.50
1	A	55	TRP	CA-C-O	-5.83	114.06	120.36
1	A	183	GLN	CB-CG-CD	5.81	122.47	112.60
1	A	41	ALA	CA-C-N	5.79	128.51	120.29
1	A	41	ALA	C-N-CA	5.79	128.51	120.29
1	A	135	ALA	CB-CA-C	5.77	119.94	110.88
1	A	313	LYS	N-CA-C	5.77	118.14	108.73
1	A	104	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	124	VAL	N-CA-CB	5.74	117.27	110.55
1	A	380	ASP	N-CA-CB	-5.74	101.94	110.71
1	A	231	ARG	NE-CZ-NH1	5.73	127.23	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	GLY	N-CA-C	-5.73	105.56	112.49
1	A	262	GLU	CA-CB-CG	5.73	125.56	114.10
1	A	101	THR	CA-C-O	-5.72	114.99	121.00
1	A	414	VAL	CA-CB-CG1	5.72	120.12	110.40
1	A	56	THR	CA-C-O	-5.71	114.53	120.70
1	A	130	ARG	N-CA-C	-5.71	105.19	111.82
1	A	291	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	A	240	ARG	CA-C-O	-5.68	114.53	120.55
1	A	162	ILE	N-CA-C	-5.67	104.82	111.00
1	A	286	GLU	N-CA-CB	5.66	118.27	110.07
1	A	364	ARG	N-CA-CB	5.64	118.25	110.07
1	A	292	PHE	N-CA-CB	5.64	119.14	110.79
1	A	192	THR	CA-C-O	-5.63	115.34	121.87
1	A	276	GLU	N-CA-CB	5.63	118.77	110.33
1	A	318	ILE	CB-CG1-CD1	5.62	125.61	113.80
1	A	287	GLU	CA-C-N	5.62	128.86	120.31
1	A	287	GLU	C-N-CA	5.62	128.86	120.31
1	A	208	ILE	N-CA-CB	5.62	117.50	110.47
1	A	54	VAL	CA-C-O	-5.62	116.07	121.63
1	A	320	LEU	O-C-N	5.59	126.31	121.34
1	A	384	ALA	O-C-N	5.59	125.83	121.47
1	A	211	ARG	CA-CB-CG	5.58	125.25	114.10
1	A	239	LYS	N-CA-C	-5.54	104.47	111.11
1	A	258	SER	CA-C-O	-5.54	115.01	120.82
1	A	90	ARG	NE-CZ-NH1	5.51	127.01	121.50
1	A	340	PHE	CA-CB-CG	5.51	119.31	113.80
1	A	251	ASP	CA-CB-CG	-5.50	107.10	112.60
1	A	163	PHE	N-CA-C	-5.50	104.93	111.69
1	A	283	ALA	CA-C-O	5.50	126.38	120.55
1	A	255	ASN	O-C-N	5.49	127.94	122.12
1	A	40	GLU	CB-CG-CD	5.47	121.91	112.60
1	A	171	GLU	CA-C-O	5.45	126.52	120.63
1	A	271	ARG	NE-CZ-NH1	5.45	126.95	121.50
1	A	400	GLN	CB-CA-C	5.43	120.08	110.85
1	A	270	HIS	N-CA-CB	5.42	118.28	110.20
1	A	361	HIS	CA-C-O	5.42	126.16	120.42
1	A	106	PRO	N-CD-CG	-5.40	97.32	103.80
1	A	207	ILE	N-CA-CB	5.40	116.50	110.62
1	A	126	LYS	N-CA-CB	5.38	117.96	109.94
1	A	403	PRO	CB-CA-C	-5.37	105.70	111.56
1	A	279	GLU	CA-C-N	5.36	130.78	122.26
1	A	279	GLU	C-N-CA	5.36	130.78	122.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	GLU	CA-C-N	5.35	128.85	120.82
1	A	107	GLU	C-N-CA	5.35	128.85	120.82
1	A	49	ASN	CA-C-N	-5.35	117.54	123.43
1	A	49	ASN	C-N-CA	-5.35	117.54	123.43
1	A	311	GLN	CA-C-O	-5.35	114.56	120.60
1	A	338	VAL	CB-CA-C	5.34	117.33	111.08
1	A	349	THR	CA-CB-CG2	5.34	119.58	110.50
1	A	88	ILE	N-CA-CB	-5.34	103.73	111.21
1	A	411	THR	CA-CB-CG2	5.34	119.58	110.50
1	A	108	GLN	CB-CA-C	5.30	119.55	110.74
1	A	358	LEU	O-C-N	5.30	128.19	122.15
1	A	56	THR	O-C-N	5.28	130.09	123.23
1	A	286	GLU	CA-C-O	-5.27	115.27	120.70
1	A	119	VAL	O-C-N	-5.26	116.94	122.20
1	A	381	PHE	CA-C-O	-5.26	115.79	121.36
1	A	151	THR	N-CA-CB	5.25	117.57	109.91
1	A	237	GLU	CA-C-O	5.25	126.03	120.10
1	A	39	GLN	CA-CB-CG	5.22	124.55	114.10
1	A	405	VAL	CA-CB-CG1	5.22	119.28	110.40
1	A	128	GLU	N-CA-CB	5.20	118.57	109.72
1	A	303	SER	N-CA-C	5.19	116.70	108.96
1	A	381	PHE	CA-CB-CG	5.18	118.98	113.80
1	A	283	ALA	O-C-N	-5.18	116.63	122.12
1	A	256	PHE	CA-C-O	-5.17	115.07	120.55
1	A	234	THR	N-CA-CB	5.16	118.29	110.45
1	A	257	LEU	CA-C-N	5.16	127.14	120.44
1	A	257	LEU	C-N-CA	5.16	127.14	120.44
1	A	209	GLU	N-CA-CB	5.13	119.16	110.49
1	A	204	LEU	CA-C-N	5.13	131.62	122.13
1	A	204	LEU	C-N-CA	5.13	131.62	122.13
1	A	143	ARG	CA-C-N	5.12	124.79	119.56
1	A	143	ARG	C-N-CA	5.12	124.79	119.56
1	A	254	VAL	CA-CB-CG1	5.11	119.09	110.40
1	A	89	PRO	CA-C-N	5.11	131.30	121.54
1	A	89	PRO	C-N-CA	5.11	131.30	121.54
1	A	14	LEU	O-C-N	5.11	126.39	121.28
1	A	379	PRO	CB-CA-C	-5.10	104.17	111.62
1	A	48	SER	CA-C-O	-5.10	115.12	120.63
1	A	195	GLU	CG-CD-OE2	5.10	130.13	118.40
1	A	59	ASN	CA-CB-CG	5.09	117.69	112.60
1	A	273	GLU	CB-CG-CD	5.08	121.23	112.60
1	A	255	ASN	CA-C-O	-5.08	115.17	120.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	SER	O-C-N	5.07	127.50	122.12
1	A	173	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	365	ARG	N-CA-CB	5.06	118.02	110.22
1	A	143	ARG	NE-CZ-NH1	5.06	126.56	121.50
1	A	277	ARG	CA-C-N	5.05	124.71	119.56
1	A	277	ARG	C-N-CA	5.05	124.71	119.56
1	A	347	HIS	CA-C-O	-5.01	115.95	121.31
1	A	50	VAL	N-CA-C	5.00	113.35	107.89
1	A	41	ALA	O-C-N	5.00	127.22	122.07

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Sidechain
1	A	119	VAL	Mainchain
1	A	135	ALA	Mainchain
1	A	149	ASN	Mainchain
1	A	250	LEU	Mainchain
1	A	290	ARG	Sidechain
1	A	339	ASP	Mainchain
1	A	377	ARG	Sidechain
1	A	67	ARG	Sidechain
1	A	77	ASP	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3208	0	3156	233	0
2	A	43	0	30	9	0
3	A	10	0	16	6	0
4	A	204	0	0	28	0
All	All	3465	0	3202	234	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 36.

All (234) 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:39:GLN:H	1:A:39:GLN:HE21	1.15	0.91
1:A:191:MET:HE2	1:A:196:ALA:HA	1.54	0.90
1:A:260:SER:HB3	1:A:288:LEU:HD13	1.60	0.83
1:A:178:LYS:HZ3	1:A:254:VAL:HG11	1.46	0.78
1:A:131:ILE:HG22	1:A:369:VAL:HG11	1.66	0.78
1:A:159:PRO:HA	1:A:162:ILE:HD12	1.67	0.77
1:A:181:THR:HG23	1:A:247:VAL:HG22	1.67	0.75
1:A:39:GLN:H	1:A:39:GLN:NE2	1.85	0.74
1:A:114:LEU:O	1:A:117:GLN:HB2	1.90	0.72
1:A:281:ILE:HG22	1:A:368:ILE:HG23	1.72	0.71
1:A:319:LEU:HG	1:A:321:PRO:HD3	1.72	0.70
1:A:177:LEU:HD13	1:A:246:LEU:HD11	1.73	0.70
1:A:203:TYR:O	1:A:206:PRO:HD2	1.91	0.70
1:A:143:ARG:NH2	1:A:413:ALA:HB2	2.06	0.70
1:A:322:GLN:HB3	1:A:348:THR:O	1.92	0.69
1:A:82:SER:O	1:A:300:ILE:HG22	1.94	0.68
1:A:407:ASP:HB3	1:A:410:THR:HG23	1.74	0.68
1:A:281:ILE:CG2	1:A:368:ILE:HG23	2.24	0.68
1:A:114:LEU:HD23	1:A:241:MET:HE1	1.76	0.68
1:A:156:GLU:HB2	1:A:157:PRO:HD3	1.76	0.67
1:A:178:LYS:NZ	1:A:254:VAL:HG11	2.09	0.67
1:A:261:MET:HE2	1:A:264:LEU:HD12	1.77	0.67
1:A:291:ARG:HH11	1:A:291:ARG:HG3	1.59	0.67
1:A:82:SER:HB2	4:A:581:HOH:O	1.96	0.65
1:A:362:LEU:O	1:A:366:GLU:HG3	1.96	0.65
1:A:128:GLU:HA	1:A:131:ILE:HD12	1.78	0.65
1:A:143:ARG:HB3	1:A:144:PRO:HD3	1.79	0.65
1:A:134:LEU:HB2	4:A:590:HOH:O	1.97	0.64
1:A:78:TYR:CE2	1:A:105:PRO:HG2	2.32	0.64
1:A:233:ILE:HG12	1:A:234:THR:O	1.97	0.64
1:A:149:ASN:C	1:A:149:ASN:HD22	2.05	0.64
1:A:229:ASN:O	1:A:231:ARG:HG3	1.98	0.63
1:A:169:LEU:HD13	1:A:203:TYR:OH	1.99	0.63
1:A:146:GLY:HA2	1:A:406:TRP:CE2	2.34	0.62
1:A:80:HIS:O	1:A:301:LEU:HA	1.98	0.62
1:A:186:ARG:HH12	1:A:255:ASN:ND2	1.97	0.62
1:A:142:LEU:HD22	1:A:148:CYS:HB3	1.81	0.61
1:A:143:ARG:HG3	1:A:411:THR:HG21	1.82	0.61
1:A:252:THR:HB	2:A:415:HEM:HBB2	1.83	0.61
1:A:303:SER:HA	1:A:314:LYS:HB2	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ARG:HH21	1:A:413:ALA:HB2	1.65	0.60
1:A:14:LEU:HD11	1:A:18:VAL:CG1	2.32	0.60
1:A:56:THR:O	1:A:61:GLY:HA2	2.01	0.60
1:A:376:THR:HG22	1:A:414:VAL:HG21	1.82	0.60
1:A:197:LYS:HE3	1:A:201:TYR:HE2	1.66	0.60
1:A:234:THR:OG1	1:A:237:GLU:HG3	2.02	0.59
1:A:208:ILE:HD12	1:A:239:LYS:HA	1.83	0.59
1:A:14:LEU:HD21	1:A:18:VAL:O	2.02	0.59
1:A:177:LEU:HD21	1:A:203:TYR:CE1	2.38	0.59
1:A:25:ASP:OD1	1:A:57:ARG:HB2	2.02	0.59
1:A:29:TYR:O	1:A:30:ASN:HB2	2.03	0.59
1:A:381:PHE:HD2	1:A:404:LEU:HD13	1.68	0.58
1:A:151:THR:HA	1:A:155:ALA:HB3	1.86	0.58
1:A:254:VAL:HG12	4:A:571:HOH:O	2.02	0.57
1:A:97:ASP:O	1:A:240:ARG:HD2	2.04	0.57
1:A:169:LEU:HD21	1:A:207:ILE:HG21	1.84	0.57
1:A:109:ARG:HB2	4:A:623:HOH:O	2.04	0.57
1:A:99:ILE:HG23	1:A:103:MET:CE	2.35	0.57
1:A:170:PRO:HG2	1:A:173:ASP:OD2	2.05	0.57
1:A:205:ILE:HD11	1:A:239:LYS:CD	2.34	0.57
1:A:407:ASP:HB3	1:A:410:THR:CG2	2.34	0.56
1:A:15:PRO:HG2	1:A:18:VAL:HG23	1.86	0.56
1:A:186:ARG:HH12	1:A:255:ASN:HD21	1.53	0.56
1:A:259:PHE:HB3	1:A:292:PHE:CD2	2.41	0.56
1:A:151:THR:OG1	1:A:401:ALA:HA	2.06	0.56
1:A:20:GLU:HA	1:A:23:VAL:HG23	1.88	0.56
1:A:186:ARG:NH1	1:A:255:ASN:ND2	2.54	0.55
1:A:319:LEU:O	1:A:320:LEU:HD23	2.06	0.55
1:A:278:PRO:C	1:A:280:ARG:H	2.14	0.55
1:A:290:ARG:HD3	1:A:345:VAL:HG13	1.89	0.55
1:A:234:THR:HB	4:A:604:HOH:O	2.07	0.55
1:A:149:ASN:C	1:A:149:ASN:ND2	2.65	0.55
1:A:332:ASN:HA	4:A:693:HOH:O	2.06	0.55
1:A:159:PRO:HG3	1:A:254:VAL:HG22	1.88	0.55
1:A:51:PRO:HB2	1:A:54:VAL:HG13	1.89	0.54
1:A:376:THR:CG2	1:A:414:VAL:HG21	2.37	0.54
3:A:416:ADM:H5	4:A:801:HOH:O	2.07	0.54
1:A:381:PHE:CD2	1:A:404:LEU:HD13	2.43	0.54
1:A:268:PRO:HB3	1:A:271:ARG:NH2	2.23	0.54
1:A:169:LEU:HD22	1:A:207:ILE:HD13	1.90	0.53
1:A:53:LEU:HD23	1:A:310:VAL:HG21	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ASP:O	1:A:331:GLU:HB2	2.08	0.53
1:A:358:LEU:HD12	2:A:415:HEM:HMD3	1.90	0.53
1:A:205:ILE:HB	1:A:206:PRO:HD3	1.91	0.53
1:A:302:THR:O	1:A:314:LYS:HE3	2.09	0.53
1:A:67:ARG:HB3	4:A:541:HOH:O	2.08	0.53
1:A:205:ILE:HD11	1:A:239:LYS:HD3	1.91	0.52
1:A:303:SER:HA	1:A:314:LYS:CB	2.39	0.52
1:A:31:PRO:HB2	1:A:41:ALA:HB1	1.91	0.52
1:A:322:GLN:HG2	1:A:351:GLY:HA2	1.91	0.52
1:A:67:ARG:NH1	1:A:328:ASP:OD1	2.42	0.52
1:A:160:ILE:O	1:A:164:MET:HG2	2.10	0.52
1:A:87:PHE:HB2	1:A:93:GLY:HA2	1.92	0.51
1:A:99:ILE:HD11	1:A:237:GLU:HA	1.93	0.51
1:A:39:GLN:HE21	1:A:39:GLN:N	1.95	0.51
1:A:99:ILE:HG23	1:A:103:MET:SD	2.50	0.51
1:A:163:PHE:CE1	1:A:246:LEU:HD22	2.45	0.51
1:A:181:THR:HG23	1:A:247:VAL:HG13	1.93	0.51
1:A:393:SER:HB3	4:A:528:HOH:O	2.09	0.51
1:A:49:ASN:HD22	1:A:49:ASN:H	1.59	0.51
1:A:140:GLU:OE2	1:A:143:ARG:NH2	2.39	0.51
1:A:349:THR:HG23	4:A:536:HOH:O	2.11	0.51
1:A:252:THR:HG21	2:A:415:HEM:C1B	2.46	0.51
1:A:15:PRO:HG2	1:A:18:VAL:CG2	2.41	0.50
1:A:69:GLN:HB3	4:A:580:HOH:O	2.10	0.50
1:A:185:THR:C	1:A:187:PRO:HD3	2.36	0.50
1:A:192:THR:OG1	1:A:195:GLU:HG2	2.10	0.50
1:A:87:PHE:HZ	3:A:416:ADM:H81	1.77	0.50
1:A:159:PRO:HG2	1:A:160:ILE:H	1.77	0.50
1:A:363:ALA:HB1	2:A:415:HEM:HAB	1.93	0.50
1:A:263:PHE:CE2	1:A:338:VAL:HG11	2.47	0.49
1:A:99:ILE:HG23	1:A:103:MET:HE3	1.94	0.49
1:A:108:GLN:HG3	1:A:355:HIS:CE1	2.48	0.49
1:A:205:ILE:CB	1:A:206:PRO:HD3	2.42	0.49
1:A:236:ASP:OD1	1:A:239:LYS:HE2	2.12	0.49
1:A:118:VAL:O	1:A:123:VAL:HG11	2.13	0.49
1:A:127:LEU:HA	4:A:587:HOH:O	2.11	0.49
1:A:181:THR:CG2	1:A:247:VAL:HA	2.41	0.49
1:A:244:LEU:HD11	3:A:416:ADM:H21	1.94	0.49
1:A:291:ARG:HG3	1:A:291:ARG:NH1	2.23	0.49
1:A:334:CYS:N	1:A:335:PRO:HD3	2.27	0.49
1:A:177:LEU:HD21	1:A:203:TYR:CD1	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLY:O	1:A:96:TYR:HB3	2.13	0.48
1:A:295:VAL:HG11	2:A:415:HEM:HMA2	1.94	0.48
1:A:15:PRO:HB2	1:A:17:HIS:CE1	2.48	0.48
1:A:174:ILE:N	1:A:175:PRO:HD2	2.28	0.48
1:A:295:VAL:HG22	1:A:396:VAL:HG22	1.94	0.48
1:A:321:PRO:CG	1:A:324:LEU:HD12	2.43	0.48
1:A:294:LEU:HD21	2:A:415:HEM:HMB3	1.96	0.48
1:A:99:ILE:HG13	1:A:240:ARG:HB3	1.95	0.48
1:A:350:PHE:O	1:A:356:LEU:HD12	2.14	0.48
1:A:22:LEU:HD22	1:A:53:LEU:O	2.14	0.48
1:A:361:HIS:HB2	4:A:560:HOH:O	2.14	0.48
1:A:56:THR:HG21	1:A:64:ILE:HD11	1.96	0.48
1:A:181:THR:HG23	1:A:247:VAL:HA	1.96	0.48
1:A:303:SER:HA	1:A:314:LYS:CG	2.43	0.48
1:A:260:SER:HB3	1:A:288:LEU:CD1	2.37	0.48
1:A:319:LEU:C	1:A:320:LEU:HD23	2.38	0.48
1:A:211:ARG:HG3	1:A:221:SER:OG	2.14	0.47
1:A:134:LEU:HD12	1:A:134:LEU:O	2.14	0.47
1:A:47:GLU:HB2	1:A:49:ASN:ND2	2.29	0.47
1:A:72:ARG:O	1:A:76:GLU:HG3	2.14	0.47
1:A:100:PRO:HG2	2:A:415:HEM:CGD	2.45	0.47
1:A:87:PHE:HE1	3:A:416:ADM:H102	1.79	0.47
1:A:274:LEU:HD12	1:A:375:LEU:HD11	1.96	0.47
1:A:197:LYS:HE3	1:A:201:TYR:CE2	2.49	0.47
1:A:53:LEU:HD23	1:A:310:VAL:CG2	2.45	0.47
1:A:287:GLU:OE1	1:A:342:ARG:HD2	2.15	0.47
1:A:297:ASP:C	1:A:319:LEU:HD12	2.40	0.47
1:A:121:MET:HB2	1:A:122:PRO:CD	2.45	0.47
1:A:151:THR:HG22	1:A:258:SER:OG	2.14	0.47
1:A:98:PHE:HB3	1:A:244:LEU:HB2	1.96	0.46
1:A:25:ASP:HB2	4:A:550:HOH:O	2.16	0.46
1:A:186:ARG:NH1	1:A:255:ASN:HD21	2.13	0.46
1:A:14:LEU:HD11	1:A:18:VAL:HB	1.98	0.46
1:A:160:ILE:HG21	1:A:174:ILE:HG12	1.98	0.46
1:A:197:LYS:HG2	1:A:201:TYR:CE2	2.50	0.46
1:A:302:THR:O	1:A:314:LYS:HG3	2.16	0.46
1:A:121:MET:HB2	1:A:122:PRO:HD3	1.98	0.46
1:A:250:LEU:O	1:A:254:VAL:HG21	2.16	0.46
1:A:91:GLU:CD	1:A:91:GLU:H	2.24	0.46
1:A:271:ARG:NH1	1:A:381:PHE:O	2.49	0.46
1:A:142:LEU:O	1:A:143:ARG:C	2.58	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:PRO:HA	4:A:681:HOH:O	2.15	0.45
1:A:357:CYS:HB2	2:A:415:HEM:C1A	2.51	0.45
1:A:143:ARG:HB3	1:A:144:PRO:CD	2.45	0.45
1:A:377:ARG:O	1:A:411:THR:HB	2.16	0.45
1:A:128:GLU:O	1:A:131:ILE:HB	2.17	0.45
1:A:188:ASP:HB2	4:A:597:HOH:O	2.16	0.45
1:A:305:TYR:O	1:A:312:LEU:N	2.47	0.45
1:A:377:ARG:NH2	1:A:414:VAL:HB	2.32	0.45
1:A:133:GLU:O	1:A:133:GLU:HG2	2.17	0.45
1:A:74:ALA:HB3	1:A:320:LEU:HD13	1.97	0.45
1:A:87:PHE:CE1	3:A:416:ADM:H102	2.51	0.45
1:A:178:LYS:HE3	1:A:182:ASP:OD1	2.16	0.45
1:A:32:SER:N	4:A:513:HOH:O	2.48	0.44
1:A:372:LYS:HD3	4:A:561:HOH:O	2.17	0.44
1:A:281:ILE:N	1:A:282:PRO:CD	2.80	0.44
1:A:407:ASP:O	1:A:408:PRO:C	2.61	0.44
1:A:391:HIS:CD2	1:A:399:VAL:HG22	2.52	0.44
1:A:85:CYS:HB3	1:A:300:ILE:HD13	2.00	0.44
1:A:132:GLN:HE22	1:A:373:GLU:CD	2.25	0.44
1:A:302:THR:HA	4:A:538:HOH:O	2.17	0.44
1:A:51:PRO:HD2	1:A:54:VAL:CG1	2.47	0.44
1:A:57:ARG:HG2	4:A:508:HOH:O	2.18	0.44
1:A:278:PRO:C	1:A:280:ARG:N	2.74	0.44
1:A:152:GLU:HB3	4:A:563:HOH:O	2.18	0.43
1:A:226:GLY:O	1:A:233:ILE:HG22	2.18	0.43
1:A:156:GLU:HB2	1:A:157:PRO:CD	2.45	0.43
1:A:161:ARG:HD2	1:A:171:GLU:OE2	2.17	0.43
1:A:99:ILE:HG22	1:A:100:PRO:HA	2.01	0.43
1:A:134:LEU:CD1	1:A:138:LEU:HD22	2.48	0.43
1:A:181:THR:HG23	1:A:247:VAL:CG2	2.42	0.43
1:A:303:SER:HA	1:A:314:LYS:HD2	2.01	0.43
1:A:17:HIS:CD2	1:A:313:LYS:HB2	2.54	0.43
1:A:252:THR:HG1	2:A:415:HEM:CHC	2.32	0.43
1:A:246:LEU:O	1:A:250:LEU:HD13	2.19	0.43
1:A:298:GLY:C	1:A:299:ARG:HG2	2.44	0.43
1:A:401:ALA:HB2	4:A:564:HOH:O	2.19	0.42
1:A:69:GLN:NE2	4:A:580:HOH:O	2.50	0.42
1:A:205:ILE:HD11	1:A:239:LYS:HD2	2.01	0.42
1:A:208:ILE:HG23	1:A:224:ALA:HB2	2.02	0.42
1:A:389:ILE:HA	4:A:659:HOH:O	2.19	0.42
1:A:61:GLY:HA3	4:A:671:HOH:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:PRO:HG2	1:A:160:ILE:N	2.35	0.42
1:A:169:LEU:CD2	1:A:207:ILE:HD13	2.50	0.42
1:A:318:ILE:HD13	1:A:320:LEU:HD21	2.01	0.42
1:A:342:ARG:HD3	4:A:643:HOH:O	2.19	0.42
1:A:171:GLU:HA	1:A:174:ILE:CD1	2.50	0.42
1:A:11:LEU:HB3	1:A:57:ARG:HB3	2.01	0.41
1:A:260:SER:CB	1:A:288:LEU:HD13	2.43	0.41
1:A:273:GLU:OE2	1:A:280:ARG:NH1	2.53	0.41
1:A:149:ASN:O	1:A:150:PHE:C	2.63	0.41
1:A:244:LEU:CD1	3:A:416:ADM:H21	2.50	0.41
1:A:278:PRO:O	1:A:280:ARG:N	2.53	0.41
1:A:78:TYR:HA	1:A:81:PHE:O	2.20	0.41
1:A:277:ARG:HB3	1:A:279:GLU:OE2	2.21	0.41
1:A:283:ALA:O	1:A:284:ALA:C	2.58	0.41
1:A:77:ASP:OD2	1:A:80:HIS:ND1	2.51	0.41
1:A:172:GLU:O	1:A:175:PRO:HD2	2.19	0.41
1:A:163:PHE:HE1	1:A:246:LEU:HD22	1.85	0.41
1:A:70:LEU:O	1:A:73:GLU:N	2.53	0.41
1:A:62:HIS:NE2	4:A:503:HOH:O	2.37	0.41
1:A:99:ILE:CD1	1:A:237:GLU:HA	2.50	0.41
1:A:149:ASN:N	1:A:153:ASP:OD2	2.54	0.41
1:A:372:LYS:HD3	4:A:545:HOH:O	2.20	0.41
1:A:290:ARG:NH2	1:A:335:PRO:O	2.52	0.40
1:A:19:PRO:HG2	1:A:22:LEU:HD12	2.03	0.40
1:A:99:ILE:O	1:A:241:MET:HG2	2.21	0.40
1:A:50:VAL:HA	1:A:51:PRO:HD3	1.88	0.40
1:A:177:LEU:HD13	1:A:246:LEU:CD1	2.46	0.40
1:A:264:LEU:O	1:A:265:ALA:C	2.64	0.40
1:A:267:SER:HA	1:A:268:PRO:HD2	1.80	0.40
1:A:164:MET:HE2	1:A:170:PRO:C	2.46	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	403/414 (97%)	351 (87%)	43 (11%)	9 (2%)	5 4

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	PHE
1	A	230	GLY
1	A	24	PHE
1	A	25	ASP
1	A	30	ASN
1	A	78	TYR
1	A	158	PHE
1	A	13	PRO
1	A	143	ARG

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	350/358 (98%)	325 (93%)	25 (7%)	13 19

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	PRO
1	A	39	GLN
1	A	49	ASN
1	A	56	THR
1	A	58	CYS
1	A	66	THR
1	A	69	GLN
1	A	79	ARG
1	A	82	SER
1	A	85	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	91	GLU
1	A	99	ILE
1	A	108	GLN
1	A	125	ASP
1	A	141	SER
1	A	211	ARG
1	A	228	VAL
1	A	246	LEU
1	A	250	LEU
1	A	258	SER
1	A	261	MET
1	A	368	ILE
1	A	369	VAL
1	A	408	PRO
1	A	414	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	46	GLN
1	A	49	ASN
1	A	59	ASN
1	A	69	GLN
1	A	108	GLN
1	A	129	ASN
1	A	149	ASN
1	A	255	ASN
1	A	272	GLN
1	A	343	GLN

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	415	1,4	50,50,50	1.33	6 (12%)	67,82,82	1.23	6 (8%)
3	ADM	A	416	-	12,12,12	1.97	5 (41%)	18,18,18	0.70	0

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	415	1,4	-	7/14/54/54	-
3	ADM	A	416	-	-	-	0/4/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	415	HEM	CAC-C3C	3.55	1.56	1.47
2	A	415	HEM	CAB-C3B	2.91	1.55	1.47
2	A	415	HEM	FE-NB	2.74	2.03	1.94
3	A	416	ADM	C4-C5	2.73	1.60	1.52
2	A	415	HEM	FE-ND	2.63	2.03	1.94
2	A	415	HEM	C3B-C2B	-2.38	1.32	1.37
2	A	415	HEM	O1D-CGD	2.26	1.29	1.22
3	A	416	ADM	C10-C3	2.24	1.58	1.52
3	A	416	ADM	C2-C1	2.19	1.58	1.52
3	A	416	ADM	C8-C1	2.15	1.58	1.52
3	A	416	ADM	C10-C7	2.06	1.58	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	415	HEM	CBD-CAD-C3D	4.50	124.99	112.53
2	A	415	HEM	CHC-C4B-NB	-3.10	121.08	124.42
2	A	415	HEM	O1D-CGD-CBD	-2.46	115.30	123.09
2	A	415	HEM	CBC-CAC-C3C	-2.43	115.39	127.53
2	A	415	HEM	CBA-CAA-C2A	2.39	119.14	112.53
2	A	415	HEM	C3B-C2B-C1B	2.31	108.14	106.41

There are no chirality outliers.

All (7) torsion outliers are listed below:

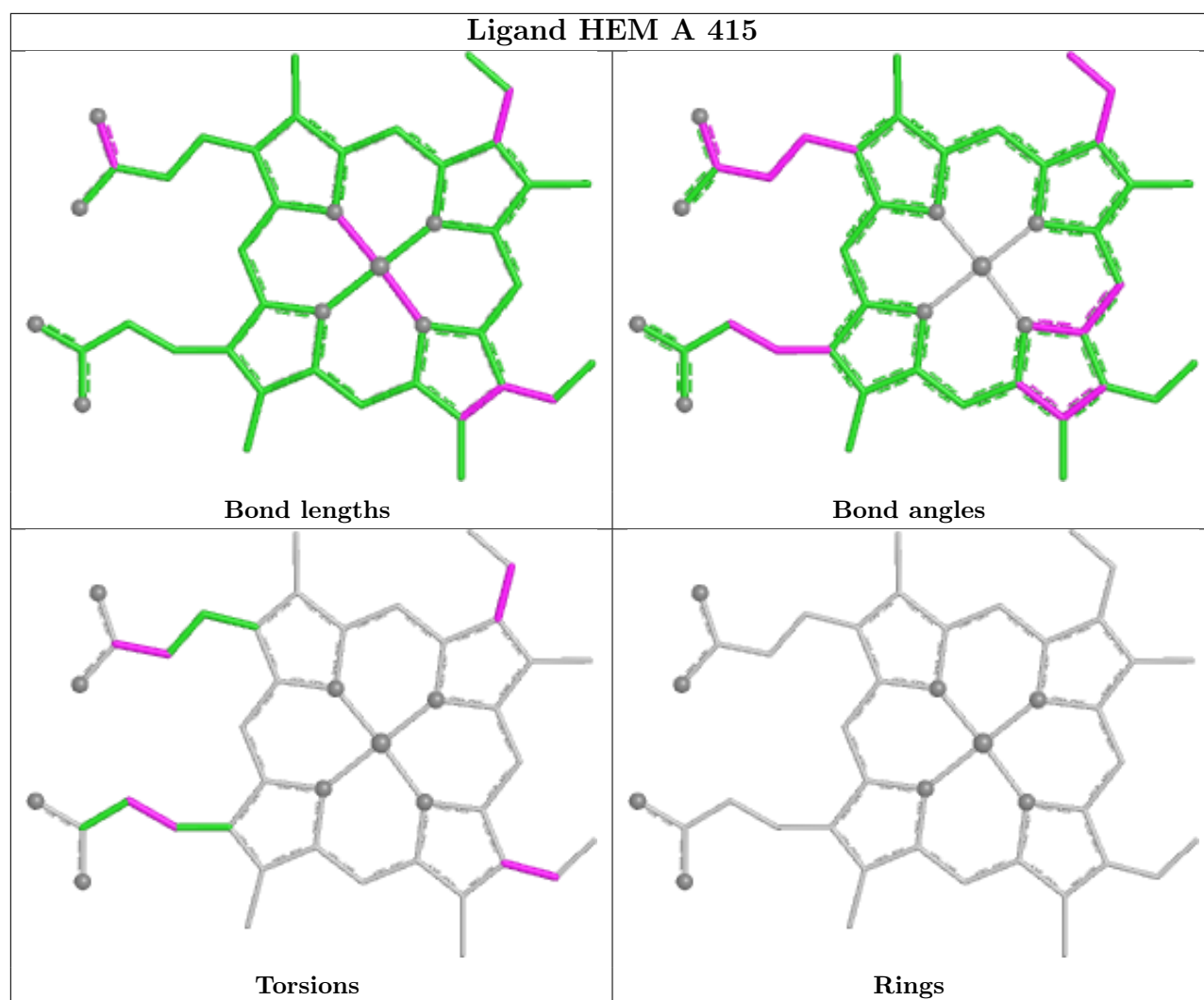
Mol	Chain	Res	Type	Atoms
2	A	415	HEM	C2B-C3B-CAB-CBB
2	A	415	HEM	C2C-C3C-CAC-CBC
2	A	415	HEM	C4C-C3C-CAC-CBC
2	A	415	HEM	C4B-C3B-CAB-CBB
2	A	415	HEM	C2A-CAA-CBA-CGA
2	A	415	HEM	CAD-CBD-CGD-O2D
2	A	415	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	415	HEM	9	0
3	A	416	ADM	6	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.