



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 08:23 PM EDT

PDB ID : 3EKB / pdb_00003ekb
Title : Crystal structure of the A264C mutant heme domain of cytochrome P450 BM3
Authors : Leys, D.
Deposited on : 2008-09-19
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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

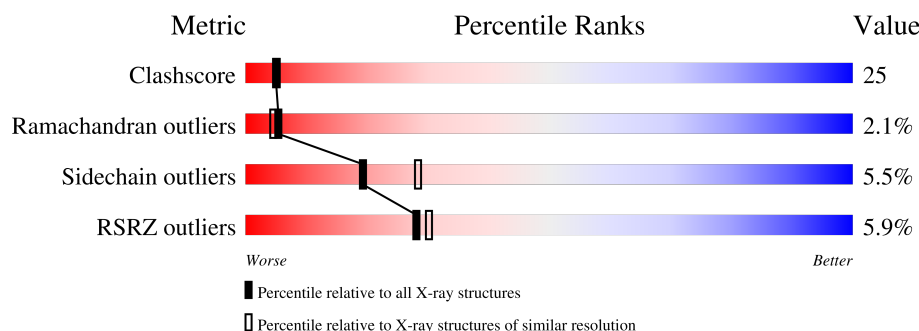
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	470	
1	B	470	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7936 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.

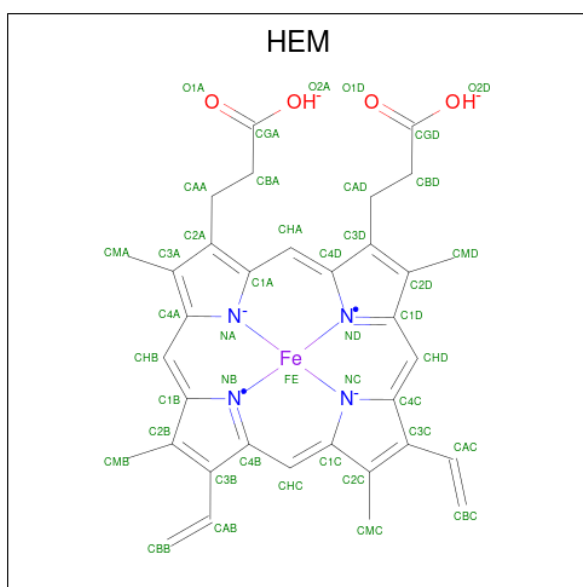
- Molecule 1 is a protein called Cytochrome P450(BM-3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	50	0
			3858	2474	653	710	21			
1	B	457	Total	C	N	O	S	0	18	0
			3698	2367	623	691	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	CYS	ALA	engineered mutation	UNP P14779
B	264	CYS	ALA	engineered mutation	UNP P14779

- 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		

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

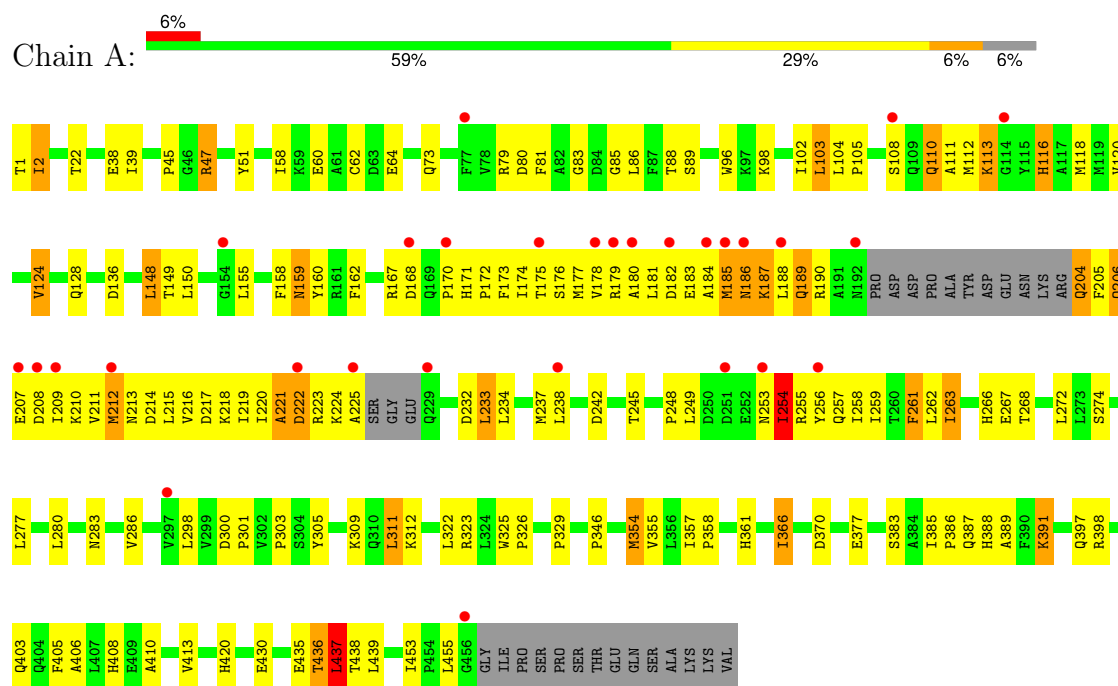
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	177	Total	O	0	0
			177	177		
3	B	117	Total	O	0	0
			117	117		

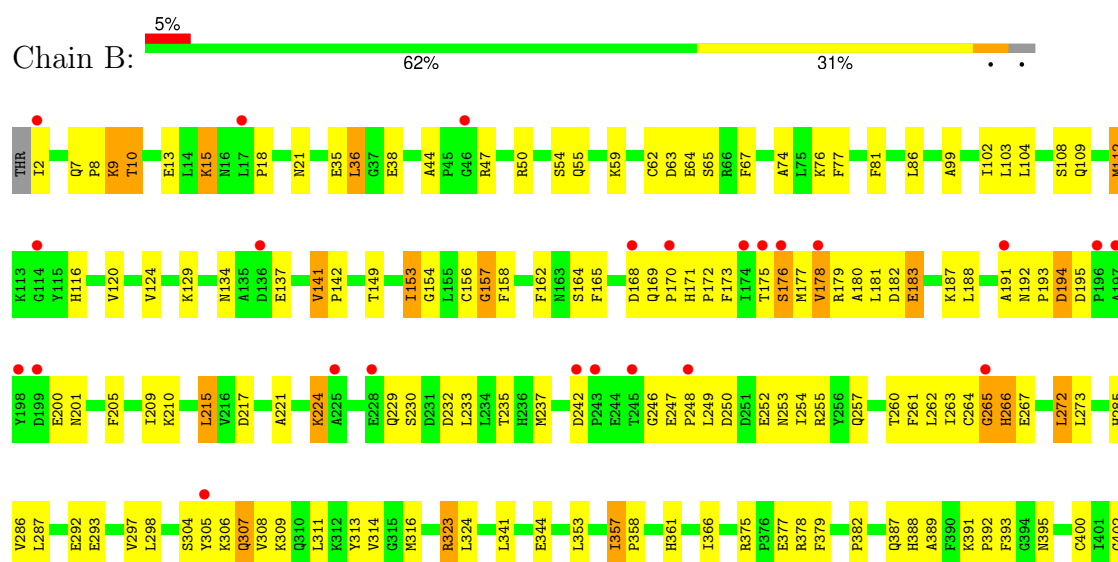
3 Residue-property plots [i](#)

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 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.

• Molecule 1: Cytochrome P450(BM-3)



• Molecule 1: Cytochrome P450(BM-3)



Q403	Q404	F405	H408	E409	A410	T411	L412	L418	K419	H420	H426	T436	L437	T438	V446	K451	T458	PRO	SER	PRO	PRO	SER	SER	THR	GLU	GLN	SER	ALA	LYS	LYS	VAL
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.88Å 118.69Å 146.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.68 – 2.30 19.68 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.68-2.30) 85.0 (19.68-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.302 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7936	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	1.26	7/3964 (0.2%)	1.23	31/5367 (0.6%)
1	B	1.26	9/3793 (0.2%)	1.29	19/5152 (0.4%)
All	All	1.26	16/7757 (0.2%)	1.26	50/10519 (0.5%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	357	ILE	CA-CB	7.90	1.58	1.54
1	A	410	ALA	N-CA	6.60	1.54	1.46
1	B	154	GLY	C-O	-6.37	1.16	1.23
1	A	124	VAL	CA-CB	5.98	1.61	1.54
1	A	405	PHE	N-CA	5.95	1.53	1.46
1	B	149	THR	CA-CB	5.93	1.62	1.53
1	B	254	ILE	C-O	-5.86	1.17	1.24
1	A	103	LEU	N-CA	5.61	1.53	1.45
1	B	411	THR	CA-CB	5.60	1.62	1.53
1	A	430	GLU	N-CA	-5.59	1.39	1.46
1	B	412	LEU	N-CA	5.56	1.52	1.46
1	B	272	LEU	CA-C	5.51	1.59	1.52
1	A	88	THR	N-CA	5.49	1.52	1.46
1	B	153	ILE	CA-CB	5.30	1.61	1.54
1	B	353	LEU	C-O	-5.23	1.17	1.23
1	A	274	SER	CA-C	5.11	1.59	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	ILE	N-CA-CB	9.41	117.79	110.45
1	A	453	ILE	CA-C-N	8.33	128.34	119.76
1	A	453	ILE	C-N-CA	8.33	128.34	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	ILE	N-CA-C	7.71	117.82	110.42
1	A	245	THR	N-CA-C	-7.26	105.34	114.56
1	A	436	THR	N-CA-C	-7.21	99.75	110.06
1	B	323	ARG	N-CA-C	-7.21	103.36	111.14
1	B	265	GLY	CA-C-N	-6.96	111.14	120.54
1	B	265	GLY	C-N-CA	-6.96	111.14	120.54
1	A	283	ASN	CA-C-N	6.83	126.63	119.05
1	A	283	ASN	C-N-CA	6.83	126.63	119.05
1	A	391	LYS	CA-C-N	-6.45	113.16	119.87
1	A	391	LYS	C-N-CA	-6.45	113.16	119.87
1	B	157	GLY	N-CA-C	6.25	122.41	114.66
1	A	437	LEU	CA-CB-CG	6.19	137.95	116.30
1	A	47	ARG	N-CA-C	6.18	118.81	109.23
1	A	357	ILE	CB-CA-C	-6.16	107.82	114.35
1	B	64	GLU	N-CA-C	6.11	119.84	112.38
1	B	162	PHE	N-CA-C	-6.09	105.34	112.89
1	A	420	HIS	N-CA-C	5.98	120.58	113.28
1	B	86	LEU	N-CA-C	5.88	117.68	111.28
1	A	96	TRP	CA-CB-CG	-5.77	102.63	113.60
1	A	261	PHE	N-CA-C	5.61	117.47	111.36
1	A	311	LEU	CA-C-N	5.61	127.73	120.44
1	A	311	LEU	C-N-CA	5.61	127.73	120.44
1	A	38	GLU	N-CA-C	5.51	119.10	112.38
1	A	113	LYS	N-CA-C	-5.50	104.93	111.69
1	A	60	GLU	N-CA-C	5.49	117.70	111.11
1	A	326	PRO	N-CA-C	-5.47	101.91	110.50
1	B	405	PHE	N-CA-C	-5.45	105.26	111.14
1	A	111	ALA	N-CA-C	-5.43	105.36	111.28
1	A	89	SER	N-CA-C	5.35	118.82	110.32
1	A	128	GLN	N-CA-C	5.33	117.09	111.28
1	B	164	SER	N-CA-C	5.32	117.83	111.71
1	B	266	HIS	N-CA-C	-5.29	104.76	111.11
1	B	10	THR	N-CA-C	5.25	117.10	110.33
1	A	366	ILE	CB-CA-C	-5.25	105.61	111.80
1	A	149	THR	N-CA-C	-5.22	105.66	112.23
1	A	116	HIS	N-CA-C	5.21	116.65	111.07
1	A	385	ILE	N-CA-C	-5.20	104.16	108.63
1	B	104	LEU	N-CA-C	5.15	120.60	113.45
1	B	141	VAL	CA-C-N	-5.12	113.65	119.28
1	B	141	VAL	C-N-CA	-5.12	113.65	119.28
1	A	277	LEU	N-CA-C	5.11	116.85	111.28
1	A	325	TRP	CA-C-N	5.09	126.49	120.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	TRP	C-N-CA	5.09	126.49	120.23
1	B	324	LEU	CA-C-N	-5.08	116.91	123.16
1	B	324	LEU	C-N-CA	-5.08	116.91	123.16
1	B	357	ILE	O-C-N	5.04	123.65	120.42
1	B	309	LYS	N-CA-C	5.00	118.84	112.34

There are no chirality outliers.

There are no planarity outliers.

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	3858	0	3738	246	1
1	B	3698	0	3517	125	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
3	A	177	0	0	28	0
3	B	117	0	0	14	1
All	All	7936	0	7315	373	1

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 25.

All (373) 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:183[A]:GLU:CB	1:A:205[A]:PHE:CE1	1.80	1.58
1:A:207[B]:GLU:O	1:A:211[B]:VAL:HG23	1.27	1.27
1:A:183[A]:GLU:CB	1:A:205[A]:PHE:CZ	2.21	1.24
1:B:173[A]:PHE:C	1:B:177[A]:MET:HE2	1.60	1.24
1:A:186[B]:ASN:O	1:A:187[B]:LYS:CG	1.86	1.23
1:A:186[B]:ASN:O	1:A:187[B]:LYS:HG3	1.34	1.21
1:A:183[A]:GLU:CB	1:A:205[A]:PHE:HE1	1.30	1.19
1:B:248:PRO:HD3	3:B:487:HOH:O	1.43	1.17
1:A:158[B]:PHE:CZ	1:A:219[B]:ILE:CD1	2.26	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158[B]:PHE:CZ	1:A:219[B]:ILE:HD12	1.82	1.15
1:B:179[A]:ARG:HA	1:B:182[A]:ASP:HB3	1.19	1.13
1:B:173[A]:PHE:O	1:B:177[A]:MET:HE2	1.49	1.13
1:A:81:PHE:HE1	1:A:184[B]:ALA:HB2	1.04	1.12
1:A:179[A]:ARG:CZ	1:A:204[A]:GLN:OE1	1.99	1.10
1:A:207[B]:GLU:O	1:A:211[B]:VAL:CG2	1.99	1.10
1:A:237:MET:HE1	1:A:258:ILE:CD1	1.80	1.10
1:A:213[A]:ASN:O	1:A:216[A]:VAL:N	1.86	1.06
1:B:179[A]:ARG:HA	1:B:182[A]:ASP:CB	1.86	1.05
1:A:81:PHE:CE1	1:A:184[B]:ALA:HB2	1.94	1.01
1:A:181[A]:LEU:HD22	1:A:437:LEU:HD22	1.41	1.01
1:B:388:HIS:CD2	1:B:391:LYS:HZ2	1.83	0.97
1:B:179[A]:ARG:CA	1:B:182[A]:ASP:HB3	1.94	0.96
1:A:108:SER:O	1:A:112:MET:HB2	1.65	0.96
1:A:174[B]:ILE:O	1:A:178[B]:VAL:HG23	1.67	0.94
1:B:388:HIS:HD2	1:B:391:LYS:NZ	1.65	0.94
1:A:158[B]:PHE:HZ	1:A:219[B]:ILE:HD12	1.20	0.93
1:A:158[B]:PHE:CZ	1:A:219[B]:ILE:HD13	2.01	0.92
1:A:158[B]:PHE:CE2	1:A:219[B]:ILE:HD13	2.05	0.92
1:A:177[B]:MET:HE3	1:A:263:ILE:HG12	1.50	0.91
1:A:237:MET:HE1	1:A:258:ILE:HD11	1.52	0.91
1:A:136:ASP:CB	3:A:633:HOH:O	2.18	0.90
1:A:179[A]:ARG:HB3	1:A:208[A]:ASP:OD2	1.72	0.89
1:B:388:HIS:HD2	1:B:391:LYS:HZ2	0.92	0.89
1:A:181[B]:LEU:HD12	1:A:185[B]:MET:HG2	1.55	0.89
1:A:213[A]:ASN:HA	1:A:216[A]:VAL:HG23	1.56	0.88
1:A:220[B]:ILE:O	1:A:223[B]:ARG:N	2.06	0.87
1:A:150:LEU:HD21	1:A:174[B]:ILE:HG12	1.55	0.87
1:A:173[B]:PHE:CE1	1:A:212[B]:MET:HG2	2.10	0.87
1:A:258:ILE:HA	3:A:478:HOH:O	1.73	0.87
1:B:173[A]:PHE:O	1:B:177[A]:MET:CE	2.23	0.87
1:A:262:LEU:O	1:A:266:HIS:HD2	1.56	0.86
1:A:213[A]:ASN:O	1:A:215[A]:LEU:N	2.08	0.85
1:B:177[A]:MET:HA	1:B:180[A]:ALA:HB3	1.58	0.85
1:A:237:MET:SD	3:A:634:HOH:O	2.35	0.84
1:A:186[B]:ASN:O	1:A:187[B]:LYS:HG2	1.74	0.84
1:A:177[B]:MET:O	1:A:180[B]:ALA:HB3	1.79	0.83
1:B:265:GLY:O	1:B:266:HIS:C	2.17	0.83
1:A:174[A]:ILE:HD13	3:A:486:HOH:O	1.77	0.83
1:A:186[B]:ASN:C	1:A:187[B]:LYS:HG3	2.04	0.82
1:B:169[A]:GLN:O	1:B:170[A]:PRO:O	1.98	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171[B]:HIS:CD2	3:A:639:HOH:O	2.31	0.82
1:B:9:LYS:HA	3:B:582:HOH:O	1.80	0.82
1:A:177[A]:MET:HB2	1:A:212[A]:MET:HE1	1.60	0.81
1:A:177[A]:MET:CB	1:A:212[A]:MET:HE1	2.11	0.81
1:B:176[A]:SER:O	1:B:180[A]:ALA:HB2	1.81	0.80
1:A:177[A]:MET:CG	3:A:623:HOH:O	2.29	0.80
1:A:167[B]:ARG:NH1	1:A:171[B]:HIS:HA	1.97	0.79
1:A:212[B]:MET:O	1:A:216[B]:VAL:HG23	1.82	0.79
1:A:177[B]:MET:HE2	3:A:486:HOH:O	1.83	0.79
1:A:213[A]:ASN:HA	1:A:216[A]:VAL:CG2	2.13	0.78
1:A:158[B]:PHE:CE2	1:A:219[B]:ILE:CD1	2.64	0.78
1:A:171[B]:HIS:HD2	3:A:639:HOH:O	1.64	0.78
1:B:177[A]:MET:C	1:B:179[A]:ARG:N	2.39	0.78
1:A:179[B]:ARG:HD2	1:A:208[B]:ASP:OD2	1.85	0.77
1:B:382:PRO:HG2	3:B:578:HOH:O	1.83	0.77
1:A:237:MET:HE1	1:A:258:ILE:HD13	1.65	0.77
1:B:177[A]:MET:C	1:B:179[A]:ARG:H	1.90	0.77
1:B:404:GLN:HG2	3:B:538:HOH:O	1.84	0.76
1:A:185[B]:MET:O	1:A:186[B]:ASN:C	2.26	0.76
1:B:247:GLU:HA	3:B:487:HOH:O	1.85	0.76
1:A:47:ARG:NH2	1:A:188[A]:LEU:O	2.19	0.75
1:B:173[A]:PHE:C	1:B:177[A]:MET:CE	2.53	0.75
1:B:305:TYR:C	1:B:305:TYR:CD1	2.63	0.75
1:A:177[A]:MET:HG3	3:A:623:HOH:O	1.83	0.74
1:B:55:GLN:O	1:B:59:LYS:HG2	1.88	0.74
1:A:181[B]:LEU:HG	1:A:182[B]:ASP:N	2.02	0.73
1:A:180[A]:ALA:HA	1:A:205[A]:PHE:CZ	2.24	0.73
1:A:210[A]:LYS:O	1:A:214[A]:ASP:OD1	2.06	0.73
1:A:436:THR:O	1:A:437:LEU:HB3	1.89	0.72
1:A:437:LEU:HD23	1:A:438:THR:H	1.55	0.71
1:A:102:ILE:C	3:A:517:HOH:O	2.34	0.71
1:A:190:ARG:HD3	3:A:606:HOH:O	1.91	0.71
1:A:170[B]:PRO:HB2	1:A:174[B]:ILE:HB	1.73	0.70
1:A:177[A]:MET:N	1:A:212[A]:MET:HE3	2.06	0.70
1:A:181[B]:LEU:HB2	3:A:623:HOH:O	1.91	0.70
1:B:62:CYS:HB3	1:B:395:ASN:OD1	1.91	0.70
1:B:388:HIS:CD2	1:B:391:LYS:NZ	2.50	0.70
1:A:81:PHE:HE1	1:A:184[B]:ALA:CB	1.94	0.69
1:A:221[A]:ALA:O	1:A:225[A]:ALA:N	2.24	0.69
1:A:220[B]:ILE:HB	1:A:238:LEU:HD11	1.74	0.68
1:A:181[B]:LEU:CD1	1:A:185[B]:MET:HG2	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:VAL:O	1:A:124:VAL:HG23	1.93	0.68
1:A:167[B]:ARG:HH12	1:A:171[B]:HIS:HA	1.58	0.68
1:A:403:GLN:NE2	3:A:506:HOH:O	2.25	0.68
1:A:64:GLU:OE2	1:A:397:GLN:HG2	1.93	0.67
1:A:186[B]:ASN:C	1:A:187[B]:LYS:CG	2.65	0.66
1:A:177[A]:MET:HB2	1:A:212[A]:MET:CE	2.25	0.66
1:A:237:MET:CE	1:A:258:ILE:HD11	2.26	0.66
1:A:181[A]:LEU:HD13	1:A:267:GLU:OE2	1.96	0.66
1:A:212[A]:MET:O	1:A:213[A]:ASN:O	2.13	0.66
1:B:10:THR:HB	1:B:15:LYS:HZ2	1.61	0.66
1:B:420:HIS:NE2	3:B:508:HOH:O	2.28	0.66
1:A:177[A]:MET:HG2	3:A:623:HOH:O	1.93	0.65
1:A:237:MET:HB3	1:A:254:ILE:HD12	1.79	0.65
1:A:162:PHE:HE1	1:A:215[A]:LEU:HD21	1.62	0.65
1:A:175[B]:THR:N	3:A:535:HOH:O	2.29	0.64
1:A:104:LEU:HB3	1:A:105:PRO:HD3	1.80	0.64
1:B:304:SER:OG	1:B:307:GLN:NE2	2.31	0.64
1:A:160:TYR:OH	1:A:171[B]:HIS:NE2	2.31	0.64
1:B:10:THR:HB	1:B:15:LYS:NZ	2.13	0.63
1:B:388:HIS:HA	1:B:391:LYS:HD2	1.80	0.63
1:B:8:PRO:O	1:B:9:LYS:CB	2.46	0.63
1:A:237:MET:HE3	1:A:254:ILE:HD12	1.80	0.63
1:A:213[A]:ASN:CA	1:A:216[A]:VAL:HG23	2.28	0.63
1:A:73:GLN:HB2	1:A:188[A]:LEU:HD23	1.81	0.62
1:B:103:LEU:HD13	1:B:261:PHE:HZ	1.63	0.62
1:B:177[A]:MET:O	1:B:179[A]:ARG:N	2.33	0.62
1:B:179[A]:ARG:C	1:B:182[A]:ASP:HB3	2.25	0.62
1:A:158[B]:PHE:HZ	1:A:219[B]:ILE:CD1	1.89	0.62
1:A:216[B]:VAL:HG11	1:A:258:ILE:HG13	1.83	0.61
1:A:183[A]:GLU:O	1:A:185[A]:MET:N	2.33	0.61
1:A:216[B]:VAL:C	1:A:218[B]:LYS:H	2.08	0.61
1:B:116:HIS:HD2	1:B:408:HIS:NE2	1.99	0.61
1:B:252:GLU:HG3	1:B:255:ARG:HH21	1.66	0.60
1:A:173[B]:PHE:CD1	1:A:212[B]:MET:HG2	2.36	0.60
1:A:262:LEU:O	1:A:266:HIS:CD2	2.48	0.60
1:A:162:PHE:CE1	1:A:215[A]:LEU:HD21	2.36	0.60
1:A:185[B]:MET:O	1:A:187[B]:LYS:N	2.34	0.60
1:B:205:PHE:CE2	1:B:209:ILE:HD11	2.37	0.60
1:A:103:LEU:HD22	1:A:233:LEU:HD12	1.84	0.60
1:A:158[B]:PHE:CZ	1:A:216[B]:VAL:HG13	2.37	0.60
1:A:280:LEU:HD23	1:A:286:VAL:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.84	0.59
1:A:206[A]:GLN:O	1:A:210[A]:LYS:CB	2.51	0.59
1:A:179[A]:ARG:NH2	1:A:204[A]:GLN:OE1	2.35	0.59
1:A:184[B]:ALA:O	1:A:185[B]:MET:O	2.21	0.59
1:A:173[B]:PHE:HD1	1:A:215[B]:LEU:HD23	1.67	0.59
1:B:393:PHE:HB3	1:B:400:CYS:HB3	1.83	0.59
1:A:167[B]:ARG:NH1	1:A:171[B]:HIS:CA	2.64	0.59
1:A:176[B]:SER:N	3:A:535:HOH:O	1.96	0.59
1:A:237:MET:HB3	1:A:254:ILE:CD1	2.32	0.59
1:B:266:HIS:CE1	1:B:267:GLU:HB2	2.38	0.59
1:A:436:THR:O	1:A:437:LEU:CB	2.49	0.58
1:A:158[B]:PHE:CD1	1:A:234:LEU:HD22	2.38	0.58
1:A:183[A]:GLU:O	1:A:186[A]:ASN:N	2.36	0.58
1:A:177[B]:MET:HE1	1:A:266:HIS:HE2	1.67	0.58
1:B:181[A]:LEU:HD11	1:B:263:ILE:HG23	1.85	0.58
1:B:179[A]:ARG:HA	1:B:182[A]:ASP:HB2	1.82	0.58
1:B:103:LEU:HD21	1:B:237:MET:HG2	1.85	0.58
1:B:99:ALA:HB2	1:B:249:LEU:HD21	1.86	0.58
1:B:177[A]:MET:O	1:B:181[A]:LEU:N	2.22	0.57
1:A:216[B]:VAL:HG11	1:A:258:ILE:HG21	1.87	0.57
1:A:249:LEU:HD12	1:A:254:ILE:HD11	1.85	0.57
1:B:285:HIS:HB2	3:B:506:HOH:O	2.05	0.56
1:B:436:THR:O	1:B:437:LEU:HB2	2.05	0.56
1:A:179[B]:ARG:HD3	1:A:204[B]:GLN:HG2	1.87	0.56
1:B:249:LEU:HD22	1:B:253:ASN:OD1	2.06	0.56
1:A:216[B]:VAL:CG1	1:A:258:ILE:HG21	2.37	0.55
1:A:254:ILE:O	1:A:258:ILE:HG12	2.06	0.55
1:A:220[B]:ILE:C	1:A:222[B]:ASP:N	2.63	0.55
1:A:216[B]:VAL:O	1:A:218[B]:LYS:N	2.37	0.55
1:A:221[A]:ALA:HA	1:A:224[A]:LYS:HB2	1.89	0.55
1:B:18:PRO:O	1:B:21:ASN:HB2	2.05	0.55
1:A:181[B]:LEU:CD1	1:A:185[B]:MET:CG	2.85	0.55
1:B:191:ALA:HB2	3:B:569:HOH:O	2.07	0.55
1:A:268:THR:OG1	3:A:647:HOH:O	2.04	0.54
1:A:105:PRO:HD2	3:A:517:HOH:O	2.06	0.54
1:B:242:ASP:O	1:B:246:GLY:N	2.40	0.54
1:B:286:VAL:HG13	1:B:313:TYR:OH	2.07	0.54
1:A:177[A]:MET:CB	1:A:212[A]:MET:CE	2.83	0.54
1:A:183[A]:GLU:O	1:A:184[A]:ALA:C	2.49	0.54
1:A:300:ASP:HB3	1:A:301:PRO:HD2	1.89	0.54
1:A:179[B]:ARG:CD	1:A:208[B]:ASP:OD2	2.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:MET:HE3	1:B:377:GLU:HA	1.90	0.54
1:A:220[B]:ILE:C	1:A:222[B]:ASP:H	2.16	0.54
1:A:185[A]:MET:HG3	3:A:622:HOH:O	2.07	0.53
1:A:257:GLN:O	1:A:261:PHE:HD1	1.92	0.53
1:B:81:PHE:HB3	1:B:209:ILE:HG12	1.91	0.53
1:B:298:LEU:HB2	1:B:419:LYS:HD2	1.90	0.53
1:A:213[A]:ASN:O	1:A:214[A]:ASP:C	2.51	0.53
1:A:177[A]:MET:CA	1:A:212[A]:MET:HE3	2.38	0.53
1:B:179[A]:ARG:O	1:B:182[A]:ASP:HB3	2.09	0.53
1:A:223[B]:ARG:HG3	3:A:569:HOH:O	2.09	0.53
1:B:392:PRO:HD2	3:B:565:HOH:O	2.07	0.53
1:A:150:LEU:HD21	1:A:174[B]:ILE:CG1	2.35	0.52
1:A:213[B]:ASN:HB3	1:A:255:ARG:NE	2.25	0.52
1:B:377:GLU:OE1	1:B:377:GLU:N	2.39	0.52
1:A:272:LEU:HD13	1:A:322:LEU:HG	1.92	0.52
1:B:103:LEU:HD21	1:B:237:MET:CG	2.39	0.52
1:A:179[A]:ARG:NE	1:A:204[A]:GLN:OE1	2.41	0.52
1:A:237:MET:HE1	1:A:258:ILE:CG1	2.38	0.52
1:A:220[B]:ILE:C	1:A:223[B]:ARG:H	2.16	0.52
1:B:157:GLY:C	1:B:158:PHE:CG	2.88	0.52
1:A:173[B]:PHE:C	1:A:173[B]:PHE:CD2	2.88	0.52
1:A:249:LEU:HD12	1:A:254:ILE:CD1	2.40	0.52
1:A:187[A]:LYS:HA	1:A:190:ARG:HD2	1.91	0.52
1:A:209[A]:ILE:O	1:A:211[A]:VAL:N	2.43	0.52
1:B:177[A]:MET:O	1:B:178[A]:VAL:C	2.53	0.52
1:A:103:LEU:HD22	1:A:233:LEU:CD1	2.39	0.52
1:A:98:LYS:CE	1:A:248:PRO:O	2.59	0.51
1:A:177[A]:MET:CA	1:A:212[A]:MET:CE	2.88	0.51
1:A:280:LEU:CD2	1:A:286:VAL:HG12	2.40	0.51
1:A:215[A]:LEU:O	1:A:216[A]:VAL:C	2.53	0.51
1:B:168[B]:ASP:N	3:B:580:HOH:O	1.94	0.51
1:B:272:LEU:C	1:B:272:LEU:HD12	2.35	0.51
1:B:176[A]:SER:O	1:B:180[A]:ALA:CB	2.54	0.51
1:A:81:PHE:CE1	1:A:184[B]:ALA:CB	2.79	0.51
1:B:44:ALA:HB3	1:B:47:ARG:HG3	1.93	0.51
1:A:220[B]:ILE:HA	1:A:223[B]:ARG:HB3	1.93	0.51
1:A:223[A]:ARG:CZ	1:A:234:LEU:HD23	2.41	0.51
1:A:173[B]:PHE:CZ	1:A:262:LEU:HD13	2.45	0.51
1:B:419:LYS:O	1:B:451:LYS:HD2	2.11	0.51
1:A:209[A]:ILE:C	1:A:211[A]:VAL:N	2.70	0.50
1:B:81:PHE:CE2	1:B:263:ILE:HD11	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:HIS:HD2	1:A:408:HIS:NE2	2.09	0.50
1:A:175[B]:THR:CA	3:A:535:HOH:O	2.59	0.50
1:A:366:ILE:HG21	1:A:389:ALA:HB1	1.92	0.50
1:A:183[A]:GLU:C	1:A:185[A]:MET:N	2.70	0.50
1:A:179[A]:ARG:NH1	1:A:204[A]:GLN:OE1	2.40	0.50
1:A:177[A]:MET:HG3	1:A:212[A]:MET:HE1	1.94	0.50
1:A:209[A]:ILE:C	1:A:211[A]:VAL:H	2.20	0.50
1:B:156:CYS:O	1:B:232:ASP:HB2	2.11	0.50
1:B:377:GLU:C	1:B:379:PHE:H	2.19	0.50
1:A:183[B]:GLU:CB	1:A:205[B]:PHE:HD1	2.25	0.50
1:A:183[B]:GLU:CB	1:A:205[B]:PHE:CD1	2.96	0.49
1:B:377:GLU:C	1:B:379:PHE:N	2.70	0.49
1:A:2:ILE:HG12	1:A:346:PRO:HD3	1.93	0.49
1:A:181[B]:LEU:HD12	1:A:185[B]:MET:CG	2.35	0.49
1:A:176[B]:SER:O	1:A:180[B]:ALA:HB2	2.11	0.49
1:B:55:GLN:O	1:B:59:LYS:CG	2.59	0.49
1:A:170[B]:PRO:O	1:A:171[B]:HIS:C	2.55	0.49
1:A:237:MET:CE	1:A:254:ILE:HD12	2.41	0.49
1:A:255:ARG:O	1:A:259:ILE:HG13	2.13	0.49
1:A:173[B]:PHE:HB2	1:A:215[B]:LEU:CD2	2.42	0.49
1:A:177[A]:MET:CG	1:A:212[A]:MET:HE1	2.42	0.49
1:B:38:GLU:HB3	1:B:54:SER:HB3	1.93	0.49
1:B:109:GLN:HB2	1:B:404:GLN:HG3	1.94	0.49
1:A:85:GLY:HA2	1:A:257:GLN:NE2	2.27	0.49
1:B:375:ARG:HH11	1:B:375:ARG:HG2	1.78	0.49
1:A:176[B]:SER:O	1:A:180[B]:ALA:CB	2.60	0.49
1:A:176[B]:SER:O	1:A:180[B]:ALA:N	2.38	0.49
1:B:102:ILE:O	1:B:102:ILE:HG22	2.13	0.49
1:B:177[A]:MET:HA	1:B:180[A]:ALA:CB	2.37	0.48
1:A:232:ASP:O	1:A:233:LEU:C	2.56	0.48
1:A:406:ALA:HB2	2:A:471:HEM:HHC	1.95	0.48
2:A:471:HEM:CMB	2:A:471:HEM:HBB2	2.43	0.48
1:B:194:ASP:HA	3:B:579:HOH:O	2.13	0.48
1:A:183[A]:GLU:CB	1:A:205[A]:PHE:HZ	2.11	0.48
1:A:221[A]:ALA:O	1:A:222[A]:ASP:C	2.57	0.48
1:A:207[B]:GLU:O	1:A:211[B]:VAL:CB	2.58	0.48
1:A:150:LEU:CD2	1:A:174[B]:ILE:HG12	2.37	0.48
1:B:169[A]:GLN:C	1:B:170[A]:PRO:O	2.55	0.48
1:A:220[B]:ILE:O	1:A:222[B]:ASP:N	2.46	0.48
1:B:35:GLU:HB3	1:B:36:LEU:HD23	1.95	0.48
1:A:300:ASP:HB3	1:A:301:PRO:CD	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181[B]:LEU:HD11	1:A:185[B]:MET:HG3	1.96	0.47
1:A:220[B]:ILE:HB	1:A:238:LEU:HD21	1.97	0.47
1:B:141:VAL:HB	1:B:142:PRO:HD3	1.97	0.47
1:B:304:SER:O	1:B:308:VAL:HG23	2.15	0.47
1:B:217:ASP:OD1	1:B:255:ARG:HD3	2.15	0.47
1:B:311:LEU:HB3	1:B:314:VAL:HB	1.96	0.47
1:B:387:GLN:HG2	1:B:388:HIS:ND1	2.29	0.47
1:A:162:PHE:HB3	1:A:174[B]:ILE:HD11	1.96	0.47
1:B:286:VAL:HG23	3:B:506:HOH:O	2.14	0.47
1:A:388:HIS:HD2	1:A:391:LYS:NZ	2.13	0.47
1:A:118:MET:HG2	3:A:615:HOH:O	2.15	0.46
1:B:253:ASN:O	1:B:257:GLN:HG2	2.14	0.46
1:A:58:ILE:HD13	1:A:355:VAL:HG13	1.96	0.46
1:A:204[A]:GLN:HG3	1:A:207[A]:GLU:HB3	1.97	0.46
1:A:224[A]:LYS:NZ	3:A:602:HOH:O	2.31	0.46
1:A:437:LEU:HD23	1:A:438:THR:HG23	1.98	0.46
1:B:2:ILE:HA	1:B:344:GLU:O	2.16	0.46
1:B:120:VAL:O	1:B:124:VAL:HG23	2.16	0.46
1:B:400:CYS:HB2	2:B:471:HEM:NA	2.31	0.46
1:B:76:LYS:HD3	3:B:584:HOH:O	2.15	0.46
1:B:178[A]:VAL:O	1:B:182[A]:ASP:HB2	2.14	0.46
1:A:162:PHE:HA	3:A:639:HOH:O	2.15	0.46
1:A:167[B]:ARG:NH1	1:A:171[B]:HIS:N	2.63	0.46
1:B:357:ILE:HG22	1:B:361:HIS:CE1	2.49	0.46
1:A:204[B]:GLN:HG3	1:A:208[B]:ASP:OD2	2.15	0.46
1:B:15:LYS:HZ2	1:B:15:LYS:HA	1.81	0.46
1:A:437:LEU:CD2	1:A:438:THR:HG23	2.46	0.46
1:B:323:ARG:HG2	1:B:361:HIS:HB3	1.98	0.46
1:A:81:PHE:CD1	1:A:205[B]:PHE:HZ	2.34	0.46
1:A:222[A]:ASP:O	1:A:223[A]:ARG:C	2.57	0.46
1:A:305:TYR:O	1:A:309:LYS:HG2	2.16	0.46
1:B:38:GLU:CB	1:B:54:SER:HB3	2.46	0.46
1:A:177[B]:MET:HE1	1:A:266:HIS:NE2	2.31	0.45
1:A:215[B]:LEU:HG	1:A:216[B]:VAL:N	2.30	0.45
1:B:74:ALA:HB2	1:B:188:LEU:HD11	1.98	0.45
1:A:103:LEU:HD21	1:A:237:MET:HG3	1.99	0.45
1:A:181[A]:LEU:HB3	1:A:436:THR:HB	1.99	0.45
1:A:221[A]:ALA:O	1:A:224[A]:LYS:N	2.49	0.45
1:B:436:THR:O	1:B:437:LEU:CB	2.65	0.45
1:A:329:PRO:O	1:A:358:PRO:HD3	2.17	0.44
1:A:298:LEU:HD21	1:A:311:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169[A]:GLN:O	1:B:170[A]:PRO:C	2.54	0.44
1:B:35:GLU:C	1:B:36:LEU:HD23	2.42	0.44
1:B:63:ASP:OD1	1:B:65:SER:OG	2.35	0.44
1:B:77:PHE:CD1	1:B:187:LYS:HE3	2.52	0.44
1:A:216[A]:VAL:HG22	1:A:259:ILE:HG12	1.99	0.44
1:A:216[B]:VAL:C	1:A:218[B]:LYS:N	2.74	0.44
1:A:216[B]:VAL:HA	1:A:219[B]:ILE:HD12	1.98	0.44
1:B:366:ILE:HG21	1:B:389:ALA:HB1	1.99	0.44
1:B:436:THR:C	1:B:438:THR:H	2.26	0.44
1:A:177[B]:MET:CE	3:A:486:HOH:O	2.53	0.44
1:A:220[A]:ILE:O	1:A:224[A]:LYS:HB2	2.17	0.44
1:B:129:LYS:HD2	1:B:165[A]:PHE:HD1	1.82	0.44
1:A:79:ARG:HG3	1:A:83:GLY:O	2.18	0.44
1:A:98:LYS:HE3	1:A:248:PRO:O	2.18	0.43
1:A:176[A]:SER:O	1:A:177[A]:MET:C	2.61	0.43
1:B:316:MET:CE	1:B:377:GLU:HA	2.48	0.43
1:A:22:THR:H	1:A:189:GLN:HE22	1.66	0.43
1:A:179[A]:ARG:O	1:A:182[A]:ASP:HB3	2.18	0.43
1:B:10:THR:H	1:B:10:THR:HG23	1.56	0.43
1:B:273:LEU:HD11	1:B:410:ALA:HA	2.00	0.43
1:B:418:LEU:HA	1:B:418:LEU:HD23	1.72	0.43
1:A:354:MET:HB2	1:A:354:MET:HE2	1.33	0.43
1:A:179[B]:ARG:HD3	1:A:204[B]:GLN:CG	2.49	0.43
1:A:204[A]:GLN:HE21	1:A:204[A]:GLN:HB2	1.60	0.43
1:A:223[B]:ARG:CG	3:A:569:HOH:O	2.65	0.43
1:A:254:ILE:HD13	1:A:254:ILE:HA	1.56	0.43
1:B:293:GLU:O	1:B:297:VAL:HG23	2.19	0.43
1:A:62:CYS:SG	1:A:391:LYS:HE2	2.58	0.43
1:B:305:TYR:HD1	1:B:306:LYS:N	2.17	0.42
1:A:215[B]:LEU:O	1:A:216[B]:VAL:C	2.62	0.42
1:B:35:GLU:CB	1:B:36:LEU:HD23	2.48	0.42
1:A:177[A]:MET:HE2	1:A:177[A]:MET:HB3	1.89	0.42
1:A:212[A]:MET:O	1:A:213[A]:ASN:C	2.63	0.42
1:A:220[B]:ILE:O	1:A:223[B]:ARG:HB3	2.18	0.42
1:A:253:ASN:O	1:A:256:TYR:HB2	2.19	0.42
1:B:153:ILE:HG13	3:B:553:HOH:O	2.19	0.42
1:B:173[B]:PHE:CD1	1:B:215:LEU:HD22	2.54	0.42
1:A:207[A]:GLU:O	1:A:211[A]:VAL:CG2	2.68	0.42
1:A:220[B]:ILE:HA	1:A:223[B]:ARG:CB	2.49	0.42
1:B:134:ASN:N	1:B:137:GLU:OE1	2.34	0.42
1:A:222[B]:ASP:O	1:A:225[B]:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171[A]:HIS:O	1:B:172[A]:PRO:C	2.62	0.42
1:A:73:GLN:HB2	1:A:188[A]:LEU:CD2	2.49	0.42
1:A:173[B]:PHE:HE2	1:A:177[B]:MET:SD	2.43	0.42
1:A:207[A]:GLU:O	1:A:211[A]:VAL:HG23	2.19	0.42
1:A:323:ARG:HG2	1:A:361:HIS:HB3	2.02	0.42
1:B:357:ILE:N	1:B:358:PRO:CD	2.82	0.42
1:A:377:GLU:H	1:A:377:GLU:CD	2.27	0.42
2:A:471:HEM:HBB2	2:A:471:HEM:HMB2	2.02	0.42
1:B:108:SER:O	1:B:112:MET:CE	2.68	0.42
1:A:259:ILE:HG13	1:A:259:ILE:H	1.65	0.41
1:A:98:LYS:HG3	1:A:242:ASP:HB2	2.03	0.41
1:A:116:HIS:HE1	1:A:303:PRO:O	2.04	0.41
1:A:213[A]:ASN:C	1:A:215[A]:LEU:N	2.76	0.41
1:B:260:THR:O	1:B:264:CYS:HB2	2.21	0.41
1:B:221:ALA:O	1:B:224:LYS:HG3	2.19	0.41
1:B:67:PHE:CZ	1:B:341:LEU:HD13	2.55	0.41
1:A:81:PHE:HD1	1:A:205[B]:PHE:HZ	1.69	0.41
1:A:86:LEU:O	1:A:398:ARG:NH2	2.54	0.41
1:A:184[B]:ALA:O	1:A:185[B]:MET:C	2.64	0.41
1:A:213[A]:ASN:O	1:A:215[A]:LEU:C	2.58	0.41
1:B:183:GLU:OE2	1:B:201:ASN:HB3	2.21	0.41
1:A:172[B]:PRO:O	3:A:535:HOH:O	2.22	0.41
1:A:173[B]:PHE:C	3:A:535:HOH:O	2.63	0.41
1:A:213[A]:ASN:O	1:A:215[A]:LEU:CA	2.68	0.41
1:A:104:LEU:C	1:A:104:LEU:HD12	2.45	0.41
1:A:173[A]:PHE:CE1	1:A:212[A]:MET:HE2	2.55	0.41
1:A:435:GLU:HG2	1:A:439:LEU:CD2	2.51	0.41
1:B:173[B]:PHE:CE2	1:B:262:LEU:HD13	2.56	0.41
1:B:229:GLN:NE2	1:B:229:GLN:HA	2.35	0.41
1:B:377:GLU:O	1:B:379:PHE:N	2.54	0.41
1:B:262:LEU:O	1:B:263:ILE:C	2.60	0.40
1:A:39:ILE:HA	1:A:51:TYR:O	2.22	0.40
1:A:110:GLN:H	1:A:113:LYS:HG3	1.87	0.40
1:B:402:GLY:HA3	2:B:471:HEM:C3C	2.56	0.40
1:A:181[A]:LEU:HD22	1:A:437:LEU:CD2	2.30	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168[B]:ASP:OD2	3:B:580:HOH:O[3_545]	2.09	0.11

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	484/470 (103%)	423 (87%)	43 (9%)	18 (4%)	2	1
1	B	473/470 (101%)	421 (89%)	45 (10%)	7 (2%)	8	8
All	All	957/940 (102%)	844 (88%)	88 (9%)	25 (3%)	5	3

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	185[A]	MET
1	A	185[B]	MET
1	A	186[A]	ASN
1	A	186[B]	ASN
1	A	187[A]	LYS
1	A	187[B]	LYS
1	A	217[A]	ASP
1	A	217[B]	ASP
1	A	159[A]	ASN
1	A	159[B]	ASN
1	A	189	GLN
1	A	221[A]	ALA
1	A	221[B]	ALA
1	A	233	LEU
1	A	437	LEU
1	B	250	ASP
1	B	378	ARG
1	B	9	LYS
1	B	194	ASP
1	B	193	PRO
1	B	426	HIS
1	A	263	ILE
1	B	215	LEU
1	A	386	PRO

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	405/412 (98%)	382 (94%)	23 (6%)	18	27
1	B	380/412 (92%)	355 (93%)	25 (7%)	15	21
All	All	785/824 (95%)	737 (94%)	48 (6%)	19	24

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	2	ILE
1	A	45	PRO
1	A	80	ASP
1	A	148	LEU
1	A	159[A]	ASN
1	A	159[B]	ASN
1	A	204[A]	GLN
1	A	204[B]	GLN
1	A	206[A]	GLN
1	A	206[B]	GLN
1	A	212[A]	MET
1	A	212[B]	MET
1	A	222[A]	ASP
1	A	222[B]	ASP
1	A	254	ILE
1	A	312	LYS
1	A	354	MET
1	A	370	ASP
1	A	383	SER
1	A	387	GLN
1	A	437	LEU
1	A	455	LEU
1	B	7	GLN
1	B	13	GLU
1	B	15	LYS
1	B	36	LEU

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Mol	Chain	Res	Type
1	B	50	ARG
1	B	112	MET
1	B	175[A]	THR
1	B	175[B]	THR
1	B	176[A]	SER
1	B	176[B]	SER
1	B	178[A]	VAL
1	B	178[B]	VAL
1	B	183	GLU
1	B	192	ASN
1	B	195	ASP
1	B	200	GLU
1	B	210	LYS
1	B	224	LYS
1	B	230	SER
1	B	233	LEU
1	B	235	THR
1	B	287	LEU
1	B	292	GLU
1	B	307	GLN
1	B	446	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	HIS
1	A	189	GLN
1	A	388	HIS
1	B	27	GLN
1	B	70	ASN
1	B	95	ASN
1	B	101	ASN
1	B	109	GLN
1	B	116	HIS
1	B	186	ASN
1	B	201	ASN
1	B	229	GLN
1	B	266	HIS
1	B	307	GLN
1	B	359	GLN
1	B	388	HIS
1	B	404	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	B	471	3,1	50,50,50	1.99	9 (18%)	67,82,82	1.56	12 (17%)
2	HEM	A	471	3,1	50,50,50	2.27	10 (20%)	67,82,82	1.71	10 (14%)

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	B	471	3,1	-	1/14/54/54	-
2	HEM	A	471	3,1	-	2/14/54/54	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	471	HEM	C3D-C2D	7.87	1.53	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	471	HEM	FE-NB	7.15	2.16	1.94
2	B	471	HEM	C3D-C2D	7.01	1.51	1.36
2	B	471	HEM	FE-NA	6.41	2.16	1.95
2	A	471	HEM	FE-ND	5.86	2.13	1.94
2	A	471	HEM	CAC-C3C	4.50	1.59	1.47
2	B	471	HEM	FE-NC	3.59	2.07	1.95
2	B	471	HEM	CMC-C2C	3.30	1.57	1.50
2	A	471	HEM	CMA-C3A	3.27	1.57	1.50
2	B	471	HEM	CMB-C2B	3.21	1.57	1.50
2	A	471	HEM	CMD-C2D	3.16	1.57	1.50
2	B	471	HEM	CAB-C3B	2.85	1.55	1.47
2	A	471	HEM	CMB-C2B	2.79	1.56	1.50
2	B	471	HEM	CMD-C2D	2.70	1.56	1.50
2	B	471	HEM	CMA-C3A	2.57	1.56	1.50
2	A	471	HEM	CMC-C2C	2.52	1.55	1.50
2	B	471	HEM	C4D-ND	2.36	1.44	1.40
2	A	471	HEM	CHD-C1D	-2.16	1.34	1.39
2	A	471	HEM	FE-NA	2.15	2.02	1.95

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	471	HEM	C4D-ND-C1D	5.28	111.46	105.21
2	A	471	HEM	CHD-C4C-NC	5.06	129.96	124.45
2	A	471	HEM	CBD-CAD-C3D	-4.51	100.07	112.53
2	B	471	HEM	CAD-C3D-C4D	4.42	132.40	124.70
2	B	471	HEM	C2A-C1A-NA	-4.17	105.52	110.15
2	B	471	HEM	CHC-C4B-NB	3.54	128.23	124.42
2	A	471	HEM	C3B-C4B-NB	-3.54	106.93	109.47
2	A	471	HEM	C1B-NB-C4B	3.43	109.27	105.21
2	B	471	HEM	CHD-C1D-ND	3.29	127.97	124.42
2	A	471	HEM	CHD-C4C-C3C	-3.25	119.73	125.21
2	A	471	HEM	C4B-C3B-C2B	2.84	109.89	107.28
2	B	471	HEM	C4D-ND-C1D	2.65	108.35	105.21
2	B	471	HEM	CAD-C3D-C2D	-2.49	123.21	127.87
2	B	471	HEM	C4A-NA-C1A	2.48	109.87	105.82
2	A	471	HEM	C4A-CHB-C1B	2.41	131.91	126.25
2	B	471	HEM	O2A-CGA-CBA	2.41	121.61	114.00
2	B	471	HEM	CBD-CAD-C3D	-2.25	106.33	112.53
2	A	471	HEM	CHC-C4B-NB	2.19	126.78	124.42
2	A	471	HEM	C1D-C2D-C3D	-2.15	104.72	106.98
2	B	471	HEM	C3A-C4A-NA	-2.04	106.87	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	471	HEM	CBA-CAA-C2A	-2.02	106.94	112.53
2	B	471	HEM	CHA-C1A-NA	2.00	127.49	123.86

There are no chirality outliers.

All (3) torsion outliers are listed below:

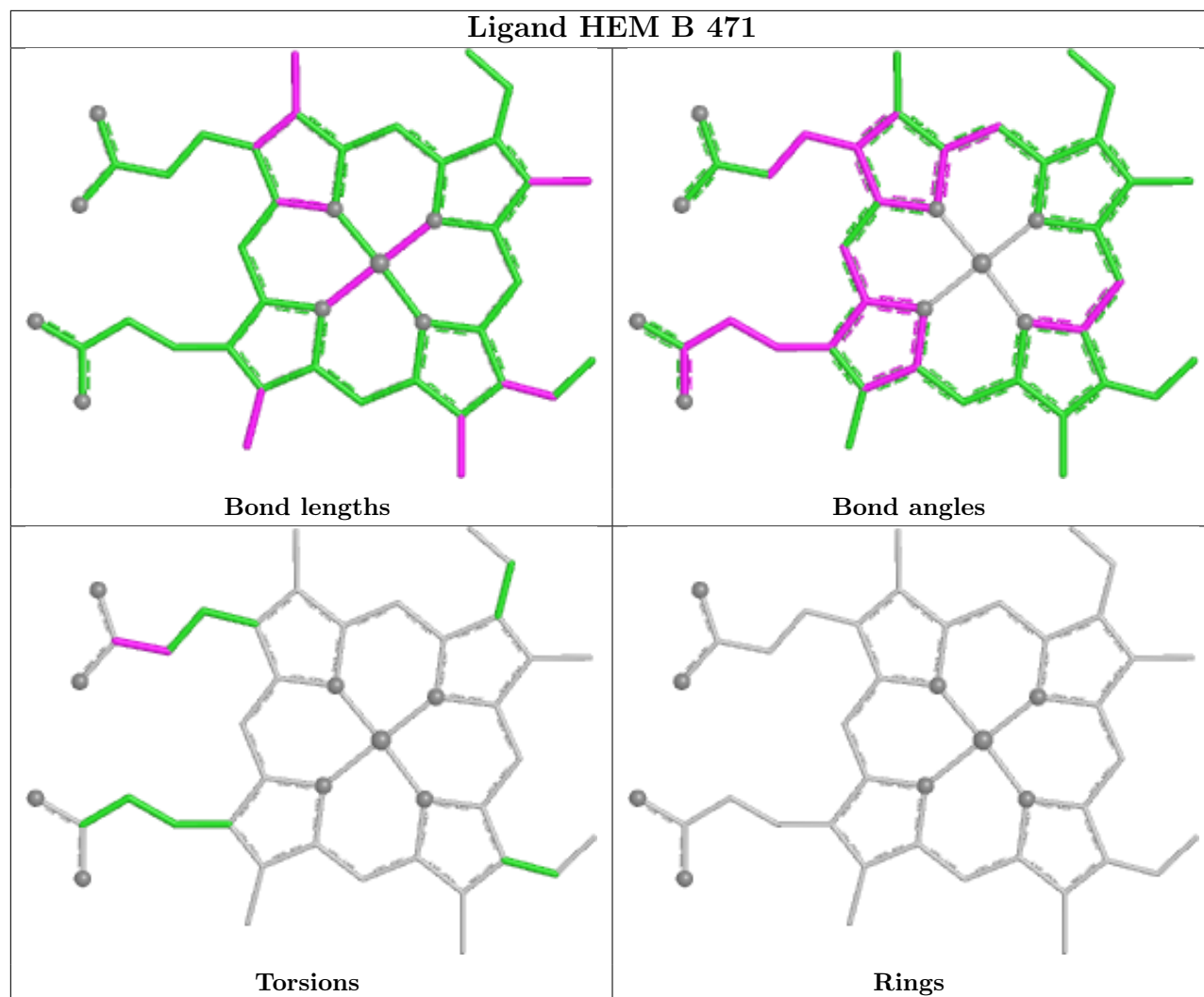
Mol	Chain	Res	Type	Atoms
2	A	471	HEM	CAD-CBD-CGD-O1D
2	A	471	HEM	CAD-CBD-CGD-O2D
2	B	471	HEM	CAD-CBD-CGD-O2D

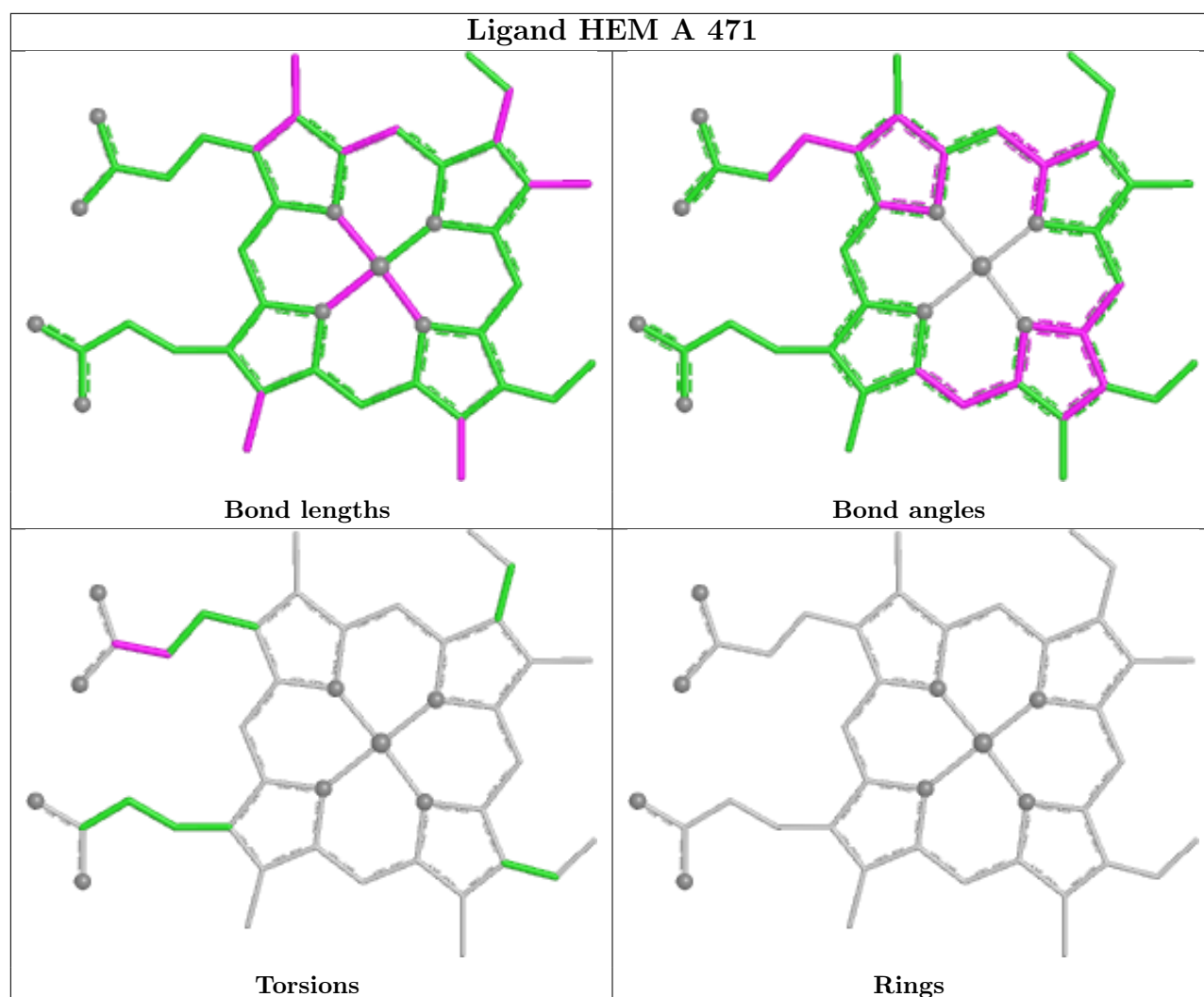
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	471	HEM	2	0
2	A	471	HEM	3	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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	442/470 (94%)	0.20	29 (6%)	24 26	14, 33, 57, 67	50 (11%)
1	B	457/470 (97%)	0.54	24 (5%)	32 34	15, 43, 68, 86	18 (3%)
All	All	899/940 (95%)	0.37	53 (5%)	28 30	14, 38, 63, 86	68 (7%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175[A]	THR	5.2
1	A	209[A]	ILE	5.2
1	B	175[A]	THR	4.5
1	B	178[A]	VAL	4.3
1	B	243	PRO	3.7
1	B	170[A]	PRO	3.6
1	A	222[A]	ASP	3.6
1	A	186[A]	ASN	3.5
1	A	170[A]	PRO	3.5
1	A	188[A]	LEU	3.3
1	A	114	GLY	3.3
1	A	225[A]	ALA	3.2
1	A	182[A]	ASP	3.2
1	B	242	ASP	3.1
1	A	456	GLY	3.0
1	A	108	SER	2.9
1	B	248	PRO	2.8
1	A	212[A]	MET	2.8
1	B	114	GLY	2.8
1	B	17	LEU	2.8
1	B	225	ALA	2.7
1	B	191	ALA	2.6
1	B	2	ILE	2.6
1	B	174[A]	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	208[A]	ASP	2.6
1	A	178[A]	VAL	2.6
1	B	196	PRO	2.6
1	B	228	GLU	2.6
1	A	256	TYR	2.5
1	A	184[A]	ALA	2.5
1	A	238	LEU	2.5
1	B	136	ASP	2.5
1	A	168[A]	ASP	2.4
1	B	198	TYR	2.4
1	A	77	PHE	2.4
1	A	251	ASP	2.3
1	B	197	ALA	2.3
1	B	265	GLY	2.3
1	B	168[A]	ASP	2.3
1	A	180[A]	ALA	2.3
1	A	192	ASN	2.2
1	B	176[A]	SER	2.2
1	A	297	VAL	2.2
1	A	253	ASN	2.2
1	A	229	GLN	2.2
1	B	305	TYR	2.2
1	A	154	GLY	2.2
1	B	46	GLY	2.2
1	A	179[A]	ARG	2.1
1	B	245	THR	2.1
1	A	185[A]	MET	2.1
1	A	207[A]	GLU	2.1
1	B	199	ASP	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

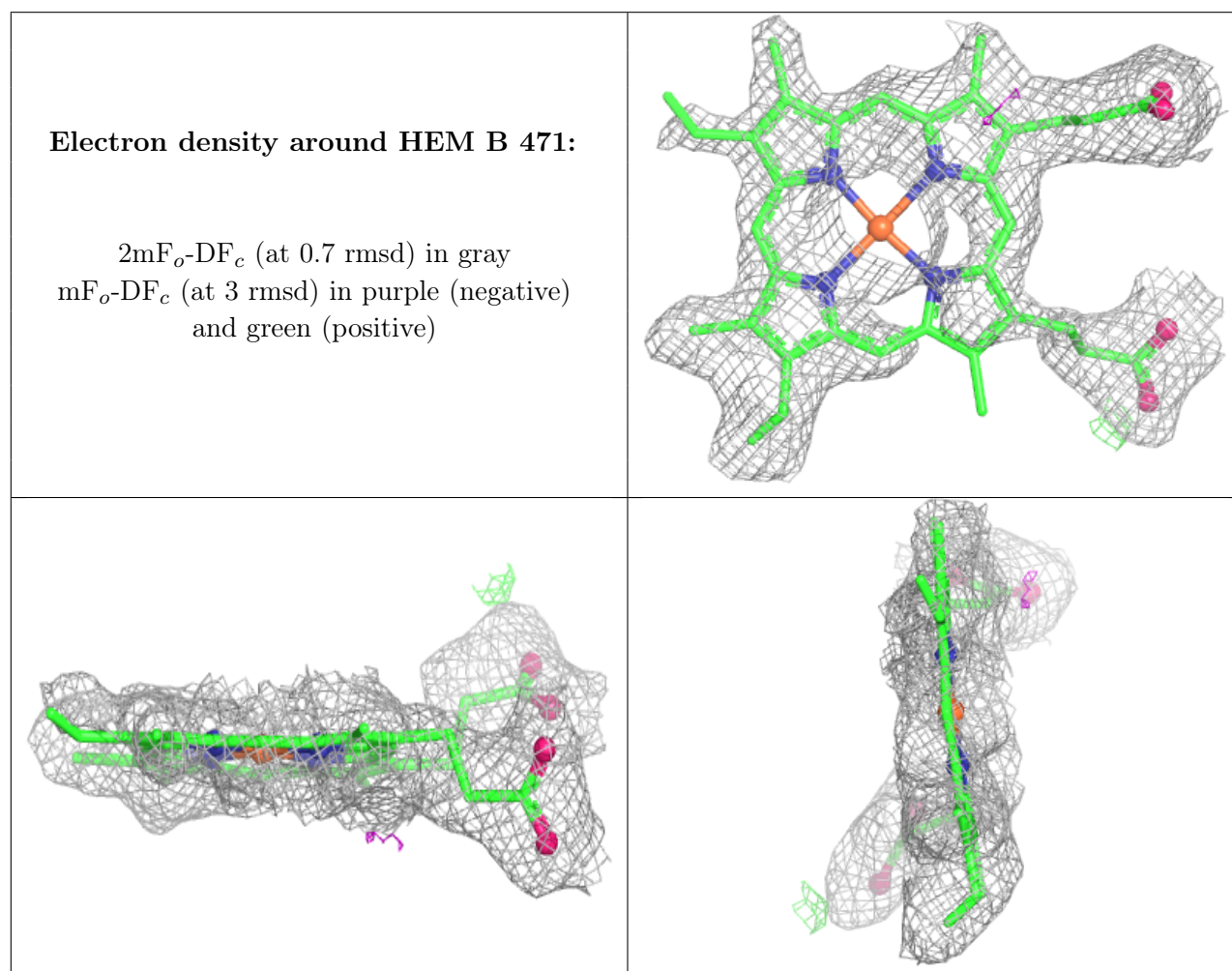
There are no oligosaccharides in this entry.

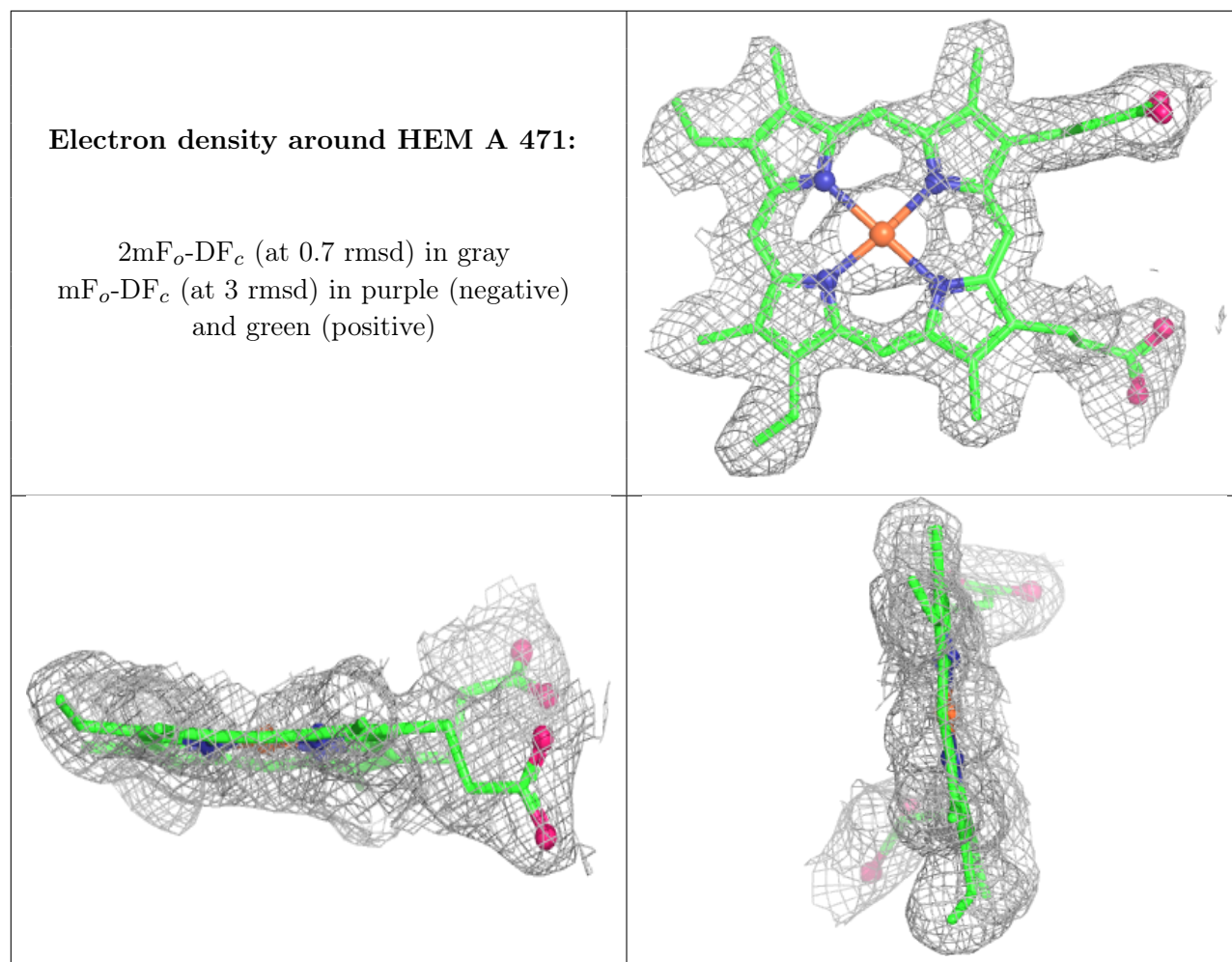
6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	B	471	43/43	0.97	0.09	27,31,35,41	0
2	HEM	A	471	43/43	0.98	0.07	17,23,26,31	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.