



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:59 AM UTC

PDB ID : 3EL3 / pdb_00003el3
Title : Distinct Monooxygenase and Farnesene Synthase Active Sites in Cytochrome P450 170A1
Authors : Zhao, B.; Waterman, M.R.
Deposited on : 2008-09-19
Resolution : 3.30 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

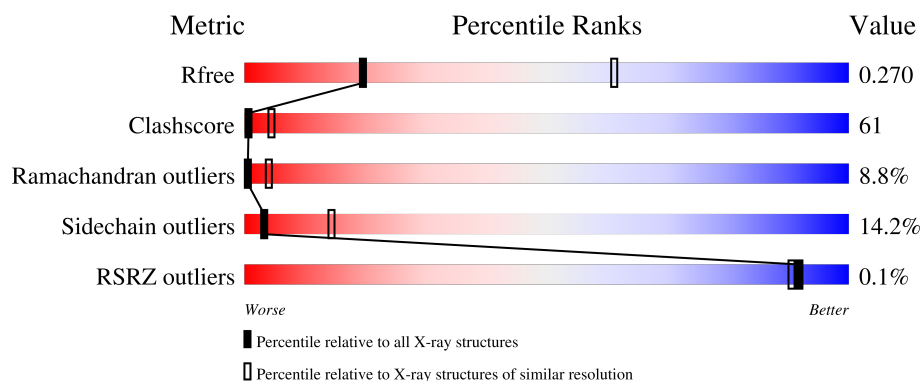
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

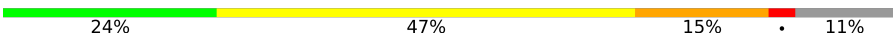
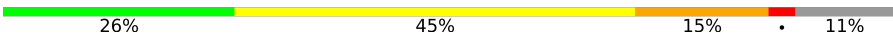
The reported resolution of this entry is 3.30 Å.

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))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	467	
1	B	467	

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	EL3	A	501	-	-	X	-
3	EL3	B	501	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6552 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.

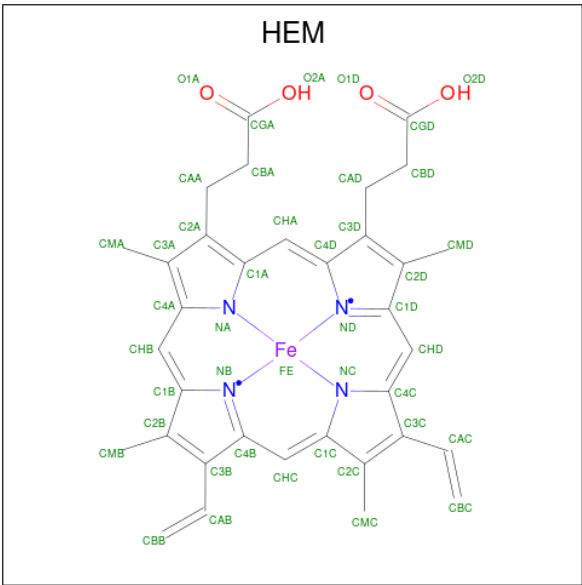
- Molecule 1 is a protein called Putative cytochrome P450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3203	2016	592	585	10			
1	B	417	Total	C	N	O	S	0	0	0
			3203	2016	592	585	10			

There are 12 discrepancies between the modelled and reference sequences:

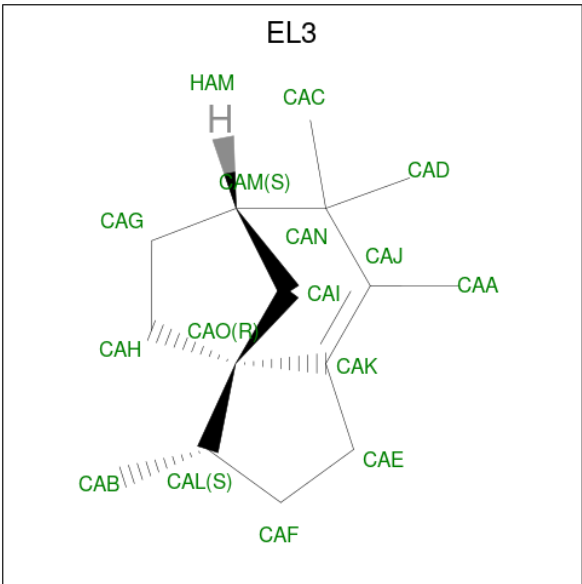
Chain	Residue	Modelled	Actual	Comment	Reference
A	462	HIS	-	expression tag	UNP Q9K498
A	463	HIS	-	expression tag	UNP Q9K498
A	464	HIS	-	expression tag	UNP Q9K498
A	465	HIS	-	expression tag	UNP Q9K498
A	466	HIS	-	expression tag	UNP Q9K498
A	467	HIS	-	expression tag	UNP Q9K498
B	462	HIS	-	expression tag	UNP Q9K498
B	463	HIS	-	expression tag	UNP Q9K498
B	464	HIS	-	expression tag	UNP Q9K498
B	465	HIS	-	expression tag	UNP Q9K498
B	466	HIS	-	expression tag	UNP Q9K498
B	467	HIS	-	expression tag	UNP Q9K498

- 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 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is (3*S*,3*aR*,6*S*)-3,7,7,8-tetramethyl-2,3,4,5,6,7-hexahydro-1*H*-3*a*,6-methanoazulene (CCD ID: EL3) (formula: C₁₅H₂₄).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			15	15		

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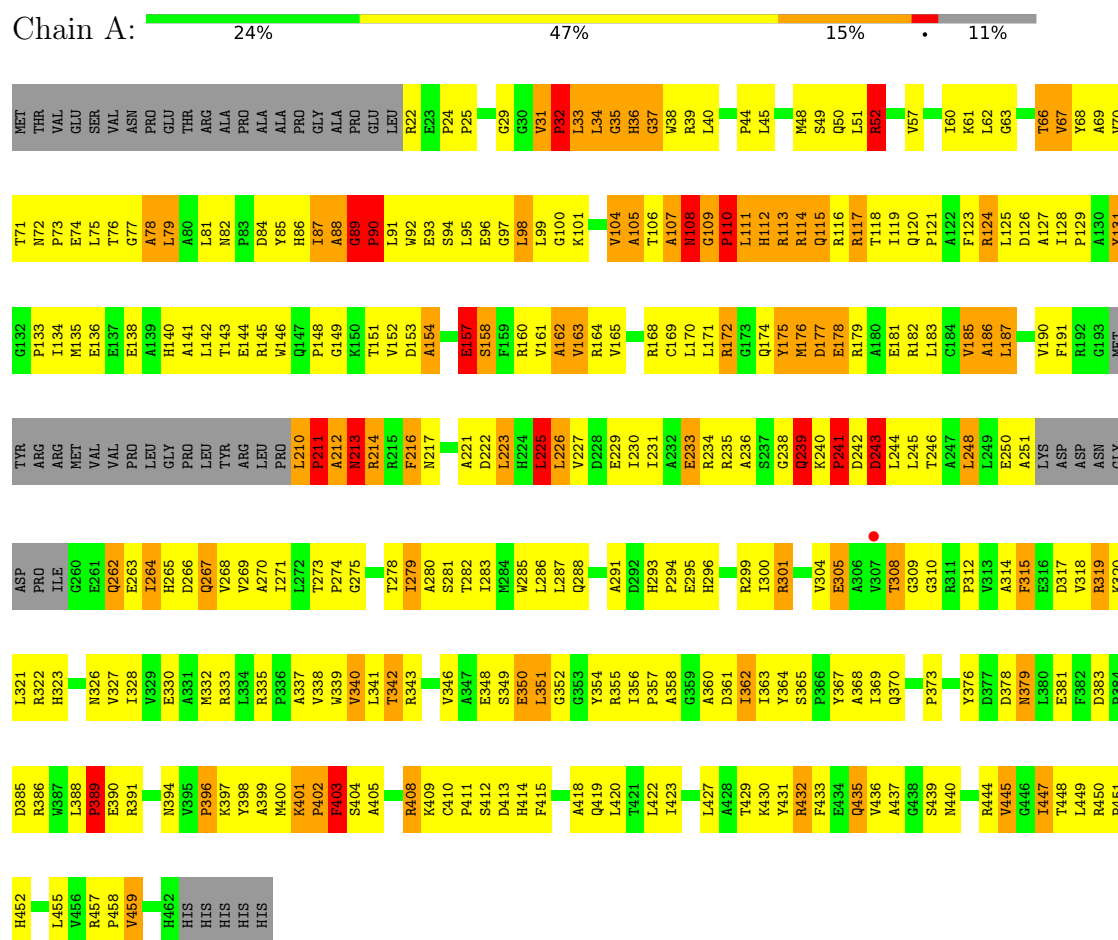
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	0	0
			15	15		
3	B	1	Total	C	0	0
			15	15		
3	B	1	Total	C	0	0
			15	15		

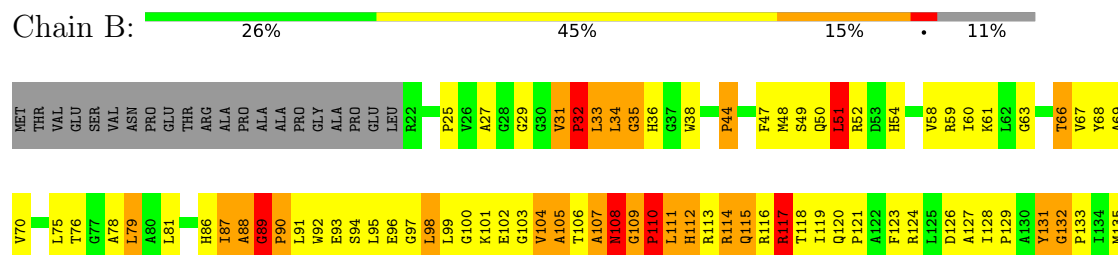
3 Residue-property plots

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 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: Putative cytochrome P450



• Molecule 1: Putative cytochrome P450



HIS	E136	VAL	VAL	E261	G325	G390	E390	HIS
HIS	E137	PRO	PRO	E262	N326	N391	R391	HIS
HIS	E138	LEU	LEU	E263	V327	I328	N394	HIS
HIS	A139	GLY	GLY	I264	I328	V329	V395	HIS
	H140	PRO	PRO	H265	V329	E330	P396	
	A141	LEU	LEU	D266	E330		K397	
	L142	TYR	TYR	Q267				
	T143	ARG	ARG	V268	R333	R333		
	E144	LEU	LEU	V269	L334	L334	M400	
	R145	PRO	PRO	A270	R335	R335	K401	
	W146	L210	L210	I271	P336	P336	P402	
	Q147	P211	P211	I272	A337	A337	F403	
	P148	A212	A212	T273	V338	V338	S404	
	G149	N213	N213	P274	W339	W339	A405	
	K150	R214	R214	G275	V340	V340	G406	
	T151	R215	R215	S276	L341	L341	K407	
	D152	F216	F216	E277	T342	T342	R408	
	W153	N217	N217	T278	R343	R343	K409	
	A154	D218	D218	I279			C410	
		A219	A219	A280	V346	V346	P411	
	E157	L220	L220	S281	A347	A347	S412	
	S158	A221	A221	T282	E348	E348	D413	
	F159	D222	D222	I283	S349	S349		
	R160	H223	H223	M284	E350	E350	S416	
	V161	H224	H224	W285	L351	L351	K417	
	A162	L225	L225	L286			A418	
	V163	L226	L226	L287	Y354	Y354		
	R164	V227	V227	Q288	R355	R355	I423	
	V165	D228	D228		I356	I356		
		E229	E229	A291	P357	P357	I427	
	G169	I230	I230		A358	A358	A428	
	L170	I231	I231	P294			T429	
	L171	A232	A232	E295	D361	D361	K430	
	R172	E233	E233	H296	I362	I362	Y431	
	G173	R234	R234	A297	I363	I363	R432	
	Q174	R235	R235	D298	Y364	Y364	F433	
	Y175	A236	A236	R299	S365	S365	F434	
	M176	S237	S237	I300	P366	P366	Q435	
	D177	G238	G238	R301	Y367	Y367	V436	
	E178	Q239	Q239	V304	A368	A368	A437	
	R179	K240	K240	E305	I369	I369	G438	
	A180	P241	P241	T308	Q370	Q370	S439	
	E181	D242	D242	G309	R371	R371	N440	
	L183	D243	D243	G310	D372	D372		
	C184	L244	L244	R311	Y376	Y376	R444	
	V185	T246	T246	V313	D377	D377	V445	
	A186	A247	A247	A314	D378	D378	G446	
	L187	L248	L248	F315	N379	N379	T447	
				E316	L380	L380	L449	
	V190	A251	A251	D317	F382	F382	R450	
	F191	LYS	LYS	V318	E381	E381	P451	
	R192	ASP	ASP	R319	D383	D383	H452	
	G193	ASN	ASN	K320	P384	P384	V456	
	MET	GLY	GLY	L321	D385	D385	R457	
	TYR	ASP	ASP	H322	R386	R386	P458	
	ARG	PRO	PRO	L323	W387	W387	V459	
	MET	ILE	ILE	L388	L388	L388		
	VAL	G250	G250	T324	P389	P389	H462	

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	107.55Å 107.55Å 141.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.48 – 3.30 35.48 – 3.30	Depositor EDS
% Data completeness (in resolution range)	83.5 (35.48-3.30) 83.4 (35.48-3.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.32Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.265 0.278 , 0.270	Depositor DCC
R_{free} test set	1010 reflections (8.61%)	wwPDB-VP
Wilson B-factor (Å ²)	87.3	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 533.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.448 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6552	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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, EL3

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	0.74	0/3273	1.33	42/4455 (0.9%)
1	B	0.73	1/3273 (0.0%)	1.37	44/4455 (1.0%)
All	All	0.74	1/6546 (0.0%)	1.35	86/8910 (1.0%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	429	THR	CA-CB	5.84	1.62	1.53

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	89	GLY	CA-C-N	13.05	136.15	119.84
1	B	89	GLY	C-N-CA	13.05	136.15	119.84
1	B	117	ARG	N-CA-C	-12.89	97.56	113.28
1	A	88	ALA	N-CA-C	-11.96	98.32	111.36
1	A	212	ALA	N-CA-C	11.89	123.91	108.34
1	A	89	GLY	CA-C-N	11.40	134.09	119.84
1	A	89	GLY	C-N-CA	11.40	134.09	119.84
1	A	117	ARG	N-CA-C	-11.03	99.55	113.23
1	B	94	SER	N-CA-C	-9.61	100.97	112.89
1	A	346	VAL	N-CA-C	-9.58	103.57	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	TYR	N-CA-C	9.49	123.76	109.25
1	B	88	ALA	N-CA-C	-9.44	100.99	111.28
1	A	78	ALA	N-CA-C	-8.85	100.23	111.02
1	A	386	ARG	N-CA-C	-8.29	103.17	113.20
1	B	386	ARG	N-CA-C	-8.25	103.21	113.28
1	A	432	ARG	N-CA-C	-8.15	94.95	108.32
1	B	175	TYR	N-CA-C	8.12	122.94	109.46
1	B	97	GLY	N-CA-C	-7.95	104.80	114.66
1	B	210	LEU	CA-C-N	7.94	129.76	119.84
1	B	210	LEU	C-N-CA	7.94	129.76	119.84
1	B	403	PHE	N-CA-C	-7.81	98.04	110.14
1	B	397	LYS	N-CA-C	7.78	119.84	111.36
1	B	213	ASN	N-CA-C	7.71	127.23	110.80
1	A	213	ASN	N-CA-C	7.68	127.16	110.80
1	B	98	LEU	N-CA-C	-7.51	104.25	113.41
1	B	395	VAL	N-CA-C	7.39	114.99	108.63
1	A	403	PHE	N-CA-C	-7.37	99.33	109.95
1	A	216	PHE	N-CA-C	-7.29	103.64	112.54
1	A	94	SER	N-CA-C	-7.23	103.44	111.82
1	A	97	GLY	N-CA-C	-7.19	103.74	113.37
1	B	216	PHE	N-CA-C	-7.14	104.44	113.01
1	B	337	ALA	N-CA-C	-6.93	102.57	111.02
1	B	268	VAL	N-CA-C	-6.86	105.07	111.45
1	A	154	ALA	N-CA-C	6.76	118.64	111.28
1	B	78	ALA	N-CA-C	-6.69	103.92	111.07
1	A	214	ARG	N-CA-C	6.66	124.99	110.80
1	B	233	GLU	N-CA-C	6.64	119.52	111.82
1	A	233	GLU	N-CA-C	6.60	118.55	111.36
1	B	405	ALA	N-CA-C	6.59	121.54	112.90
1	A	63	GLY	CA-C-N	6.53	126.30	119.05
1	A	63	GLY	C-N-CA	6.53	126.30	119.05
1	B	287	LEU	N-CA-C	-6.53	103.43	111.40
1	B	131	TYR	N-CA-C	-6.47	105.21	113.23
1	A	52	ARG	N-CA-C	6.43	118.29	111.28
1	B	427	LEU	N-CA-C	6.24	118.63	111.02
1	A	131	TYR	N-CA-C	-6.17	105.57	113.23
1	B	212	ALA	N-CA-C	6.12	123.84	110.80
1	A	172	ARG	N-CA-C	6.10	119.44	109.06
1	A	210	LEU	CA-C-N	6.08	127.43	119.84
1	A	210	LEU	C-N-CA	6.08	127.43	119.84
1	B	214	ARG	N-CA-C	6.05	123.69	110.80
1	A	110	PRO	N-CA-C	-6.02	100.07	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	GLN	N-CA-C	6.00	118.08	108.41
1	B	346	VAL	N-CA-C	-5.98	105.89	111.45
1	B	144	GLU	N-CA-C	-5.98	105.82	113.23
1	A	144	GLU	N-CA-C	-5.84	106.32	113.50
1	A	262	GLN	N-CA-C	-5.83	105.74	112.92
1	B	119	ILE	N-CA-C	5.75	116.53	110.72
1	A	36	HIS	N-CA-C	-5.69	105.83	112.89
1	B	110	PRO	CA-C-N	-5.67	116.92	123.04
1	B	110	PRO	C-N-CA	-5.67	116.92	123.04
1	B	63	GLY	CA-C-N	5.66	125.33	119.05
1	B	63	GLY	C-N-CA	5.66	125.33	119.05
1	B	407	LYS	N-CA-C	-5.64	105.65	112.54
1	A	447	ILE	N-CA-C	-5.58	104.92	110.62
1	A	157	GLU	N-CA-C	5.50	118.46	111.69
1	A	108	ASN	N-CA-C	-5.50	99.09	110.80
1	A	225	LEU	N-CA-C	-5.49	105.19	111.07
1	A	401	LYS	CA-C-N	5.46	125.55	119.32
1	A	401	LYS	C-N-CA	5.46	125.55	119.32
1	A	119	ILE	N-CA-C	5.41	116.19	110.72
1	B	161	VAL	N-CA-C	-5.38	104.33	111.05
1	A	250	GLU	N-CA-C	5.38	116.89	110.44
1	B	348	GLU	N-CA-C	-5.37	102.34	110.24
1	B	110	PRO	N-CA-C	-5.34	101.46	112.47
1	B	432	ARG	N-CA-C	-5.32	98.23	107.49
1	B	431	TYR	N-CA-C	5.29	118.79	109.80
1	B	108	ASN	N-CA-C	-5.24	99.64	110.80
1	A	71	THR	N-CA-C	5.21	118.66	112.72
1	A	390	GLU	N-CA-C	5.19	116.62	111.07
1	B	395	VAL	CA-C-N	5.13	126.25	119.84
1	B	395	VAL	C-N-CA	5.13	126.25	119.84
1	A	90	PRO	N-CA-C	5.12	123.02	112.47
1	B	281	SER	N-CA-C	-5.12	104.97	111.11
1	A	98	LEU	N-CA-C	-5.09	106.23	112.90
1	B	439	SER	N-CA-C	-5.08	103.45	110.35

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	175	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3203	0	3165	409	0
1	B	3203	0	3165	392	0
2	A	43	0	30	5	0
2	B	43	0	30	8	0
3	A	30	0	48	10	0
3	B	30	0	48	18	0
All	All	6552	0	6486	801	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 61.

All (801) 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:B:142:LEU:HD21	1:B:161:VAL:HG21	1.23	1.19
1:B:91:LEU:HB3	3:B:502:EL3:HAF	1.22	1.18
1:B:61:LYS:HG2	1:B:66:THR:HG23	1.30	1.10
1:B:79:LEU:HD11	1:B:362:ILE:HD11	1.28	1.09
1:A:91:LEU:HB3	3:A:502:EL3:HAF	1.31	1.08
1:B:92:TRP:HE1	3:B:501:EL3:HAIA	1.01	1.08
1:B:90:PRO:HG3	1:B:361:ASP:HB3	1.38	1.05
1:A:79:LEU:HD11	1:A:362:ILE:HD11	1.31	1.05
1:A:142:LEU:HD11	1:A:161:VAL:HG22	1.37	1.04
1:A:301:ARG:HB3	1:A:301:ARG:HH11	1.22	1.04
1:A:274:PRO:HB3	3:A:501:EL3:HAHA	1.38	1.03
1:A:301:ARG:HG3	1:A:429:THR:HA	1.41	1.01
1:B:29:GLY:H	1:B:36:HIS:CE1	1.77	1.01
1:A:408:ARG:HG2	1:A:408:ARG:HH11	1.25	1.01
1:B:109:GLY:HA3	1:B:408:ARG:NH2	1.75	1.00
1:B:432:ARG:HB3	1:B:459:VAL:HG22	1.42	1.00
1:B:146:TRP:HE1	1:B:157:GLU:HG2	1.27	0.99
1:A:88:ALA:O	1:A:93:GLU:HB2	1.61	0.98
1:B:142:LEU:HD11	1:B:161:VAL:HG22	1.45	0.98
1:B:76:THR:HG21	1:B:369:ILE:HD11	1.43	0.98
1:B:29:GLY:H	1:B:36:HIS:HE1	1.05	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:TRP:CZ2	3:B:501:EL3:HABB	2.00	0.96
1:A:87:ILE:N	1:A:87:ILE:HD12	1.78	0.96
1:B:90:PRO:HG3	1:B:361:ASP:CB	1.95	0.96
1:A:90:PRO:HG3	1:A:361:ASP:HB3	1.46	0.96
1:B:128:ILE:HG13	1:B:129:PRO:HD3	1.48	0.96
1:A:142:LEU:HD21	1:A:161:VAL:HG21	1.48	0.96
1:B:91:LEU:CB	3:B:502:EL3:HAF	1.96	0.96
1:B:61:LYS:HG2	1:B:66:THR:CG2	1.95	0.95
1:A:170:LEU:O	1:A:171:LEU:HD23	1.66	0.95
1:B:278:THR:HG22	2:B:500:HEM:HBB2	1.48	0.95
1:B:403:PHE:CE2	1:B:413:ASP:HA	2.03	0.94
1:B:391:ARG:HA	1:B:394:ASN:HD22	1.33	0.93
1:B:92:TRP:NE1	3:B:501:EL3:HAIA	1.84	0.93
1:A:76:THR:HG21	1:A:369:ILE:HD11	1.50	0.93
1:B:87:ILE:HD12	1:B:87:ILE:N	1.84	0.92
1:B:440:ASN:ND2	1:B:452:HIS:HB2	1.85	0.91
1:B:160:ARG:O	1:B:164:ARG:HG3	1.70	0.91
1:A:91:LEU:CB	3:A:502:EL3:HAF	1.99	0.91
1:B:170:LEU:O	1:B:171:LEU:HD23	1.71	0.91
1:B:244:LEU:HD11	1:B:271:ILE:HD13	1.50	0.90
1:A:61:LYS:HG2	1:A:66:THR:HG23	1.52	0.90
1:A:128:ILE:HG13	1:A:129:PRO:HD3	1.55	0.89
1:B:135:MET:HE1	1:B:418:ALA:HB1	1.52	0.89
1:A:36:HIS:HD2	1:A:61:LYS:H	1.21	0.88
1:A:61:LYS:HG2	1:A:66:THR:CG2	2.04	0.88
1:A:128:ILE:CG1	1:A:129:PRO:HD3	2.04	0.88
1:A:142:LEU:HD11	1:A:161:VAL:CG2	2.04	0.87
1:B:87:ILE:HG12	1:B:408:ARG:HD2	1.56	0.87
1:B:301:ARG:HG3	1:B:429:THR:HA	1.54	0.87
1:A:234:ARG:HD2	1:A:245:LEU:HD22	1.55	0.86
1:A:348:GLU:N	1:A:358:ALA:HB2	1.89	0.86
1:A:214:ARG:O	1:A:217:ASN:HB2	1.75	0.86
1:B:408:ARG:HG2	1:B:408:ARG:HH11	1.38	0.86
1:B:214:ARG:O	1:B:217:ASN:HB2	1.74	0.86
1:B:111:LEU:O	1:B:113:ARG:N	2.07	0.86
1:B:100:GLY:HA2	1:B:105:ALA:C	2.00	0.86
1:B:223:LEU:O	1:B:227:VAL:HG23	1.76	0.85
1:A:301:ARG:HB3	1:A:301:ARG:NH1	1.92	0.84
1:B:81:LEU:HD21	1:B:405:ALA:HB1	1.60	0.84
1:B:128:ILE:CG1	1:B:129:PRO:HD3	2.08	0.84
1:B:92:TRP:HZ2	3:B:501:EL3:HABB	1.38	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LEU:O	1:A:227:VAL:HG23	1.77	0.83
1:B:88:ALA:O	1:B:93:GLU:HB2	1.78	0.83
1:B:90:PRO:CG	1:B:361:ASP:HB3	2.08	0.83
1:A:90:PRO:HG3	1:A:361:ASP:CB	2.09	0.83
1:B:31:VAL:HG12	1:B:32:PRO:HD2	1.61	0.82
1:A:174:GLN:O	1:A:176:MET:HE2	1.80	0.82
1:B:92:TRP:HZ2	3:B:501:EL3:CAB	1.93	0.82
1:B:79:LEU:HD21	1:B:362:ILE:HD13	1.60	0.82
1:B:29:GLY:N	1:B:36:HIS:HE1	1.78	0.81
1:A:109:GLY:HA3	1:A:408:ARG:NH2	1.94	0.81
1:A:408:ARG:HG2	1:A:408:ARG:NH1	1.91	0.81
1:B:133:PRO:HA	1:B:136:GLU:OE1	1.78	0.81
1:A:391:ARG:O	1:A:394:ASN:HB2	1.80	0.81
1:B:179:ARG:O	1:B:183:LEU:HG	1.79	0.80
1:B:285:TRP:CZ3	1:B:335:ARG:HD2	2.16	0.80
1:A:435:GLN:HE21	1:A:439:SER:HB3	1.46	0.80
1:B:245:LEU:O	1:B:245:LEU:HD23	1.82	0.80
1:A:403:PHE:CE2	1:A:413:ASP:HA	2.17	0.80
1:B:86:HIS:NE2	1:B:110:PRO:HA	1.98	0.79
1:A:146:TRP:HE1	1:A:157:GLU:HG2	1.46	0.79
1:B:90:PRO:HD3	1:B:361:ASP:OD2	1.82	0.78
1:B:315:PHE:O	1:B:318:VAL:HG22	1.83	0.78
1:B:36:HIS:HD2	1:B:61:LYS:H	1.32	0.78
1:A:190:VAL:HG11	1:A:216:PHE:CD1	2.19	0.78
1:A:86:HIS:HD2	1:A:87:ILE:H	1.32	0.77
1:A:296:HIS:O	1:A:300:ILE:HG13	1.85	0.77
1:A:91:LEU:HB3	3:A:502:EL3:CAF	2.13	0.77
1:A:161:VAL:O	1:A:165:VAL:HG23	1.85	0.77
1:B:131:TYR:HB3	1:B:169:CYS:SG	2.25	0.77
1:A:279:ILE:HD13	2:A:500:HEM:HMC2	1.67	0.77
1:B:79:LEU:HD11	1:B:362:ILE:CD1	2.12	0.76
1:B:118:THR:O	1:B:121:PRO:HD2	1.84	0.76
1:B:187:LEU:HG	1:B:216:PHE:HE2	1.48	0.76
1:A:86:HIS:NE2	1:A:110:PRO:HA	2.00	0.76
1:A:432:ARG:HB3	1:A:459:VAL:HG22	1.68	0.76
1:A:300:ILE:HD11	1:A:327:VAL:HG21	1.67	0.76
1:B:142:LEU:HD21	1:B:161:VAL:CG2	2.12	0.76
1:B:244:LEU:HD11	1:B:271:ILE:CD1	2.16	0.76
1:A:33:LEU:HB2	1:A:34:LEU:HD23	1.68	0.75
1:A:112:HIS:O	1:A:114:ARG:N	2.18	0.75
1:A:81:LEU:HD21	1:A:405:ALA:HB1	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ILE:N	1:A:87:ILE:CD1	2.49	0.75
1:A:212:ALA:HB3	1:A:216:PHE:HD1	1.52	0.75
1:A:31:VAL:HG12	1:A:32:PRO:HD2	1.68	0.75
1:A:79:LEU:HD11	1:A:362:ILE:CD1	2.13	0.75
1:A:133:PRO:HA	1:A:136:GLU:OE1	1.86	0.75
1:B:273:THR:HB	1:B:274:PRO:HD3	1.67	0.75
1:B:348:GLU:N	1:B:358:ALA:HB2	2.02	0.75
1:A:111:LEU:O	1:A:113:ARG:N	2.19	0.74
1:A:148:PRO:HA	1:A:458:PRO:O	1.86	0.74
1:A:333:ARG:CG	1:A:370:GLN:HB3	2.17	0.74
1:B:113:ARG:O	1:B:116:ARG:N	2.21	0.74
1:A:123:PHE:HB3	1:A:411:PRO:O	1.86	0.74
1:B:143:THR:HG23	1:B:430:LYS:CD	2.18	0.74
1:A:296:HIS:HD2	1:A:323:HIS:CE1	2.06	0.74
1:B:91:LEU:HB3	3:B:502:EL3:CAF	2.10	0.74
1:B:178:GLU:HA	1:B:181:GLU:CD	2.13	0.74
1:B:388:LEU:HD12	1:B:391:ARG:HH21	1.52	0.74
1:B:114:ARG:C	1:B:116:ARG:H	1.95	0.73
1:A:49:SER:HB3	1:A:52:ARG:NH2	2.02	0.73
1:A:48:MET:HE3	1:A:365:SER:HB2	1.69	0.73
1:A:52:ARG:HH11	1:A:368:ALA:HB1	1.52	0.73
1:A:285:TRP:CZ3	1:A:451:PRO:HG3	2.23	0.73
1:B:146:TRP:NE1	1:B:157:GLU:HG2	2.02	0.73
1:B:287:LEU:HD22	1:B:456:VAL:HG21	1.71	0.73
1:A:128:ILE:HG13	1:A:129:PRO:CD	2.19	0.73
1:A:431:TYR:CD1	1:A:458:PRO:HB3	2.24	0.72
1:A:244:LEU:HD11	1:A:271:ILE:HD12	1.70	0.72
1:B:355:ARG:O	1:B:357:PRO:HD3	1.89	0.72
1:A:104:VAL:HG13	1:A:270:ALA:HB2	1.70	0.72
1:A:114:ARG:C	1:A:116:ARG:H	1.96	0.72
1:A:244:LEU:HD11	1:A:271:ILE:CD1	2.19	0.72
1:A:436:VAL:HG12	1:A:437:ALA:O	1.90	0.72
1:B:135:MET:HE1	1:B:418:ALA:CB	2.19	0.72
1:B:212:ALA:HB3	1:B:216:PHE:HD1	1.54	0.72
1:A:273:THR:HB	1:A:274:PRO:HD3	1.71	0.72
1:B:79:LEU:CD1	1:B:362:ILE:HD11	2.14	0.72
1:A:135:MET:HE1	1:A:418:ALA:HB1	1.70	0.72
1:B:87:ILE:O	1:B:87:ILE:HG22	1.89	0.72
1:B:87:ILE:CG1	1:B:408:ARG:HD2	2.19	0.71
1:B:128:ILE:HG13	1:B:129:PRO:CD	2.21	0.71
1:B:112:HIS:CD2	1:B:113:ARG:N	2.58	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:HIS:O	1:B:327:VAL:HG23	1.89	0.71
1:B:96:GLU:HA	1:B:99:LEU:CB	2.21	0.71
1:B:138:GLU:O	1:B:141:ALA:HB3	1.91	0.71
1:B:104:VAL:HG13	1:B:270:ALA:HB2	1.73	0.70
1:B:432:ARG:HB3	1:B:459:VAL:CG2	2.21	0.70
1:B:112:HIS:O	1:B:114:ARG:N	2.24	0.70
1:B:403:PHE:HD2	1:B:410:CYS:HB3	1.56	0.70
1:B:408:ARG:HG2	1:B:408:ARG:NH1	1.99	0.70
1:A:183:LEU:O	1:A:187:LEU:HB2	1.92	0.70
1:B:305:GLU:HA	1:B:308:THR:HG22	1.72	0.70
1:A:323:HIS:O	1:A:327:VAL:HG23	1.92	0.70
1:B:391:ARG:O	1:B:394:ASN:HB2	1.90	0.70
1:A:29:GLY:H	1:A:36:HIS:CE1	2.10	0.70
1:A:187:LEU:HG	1:A:216:PHE:CE2	2.27	0.69
1:B:175:TYR:HB3	1:B:177:ASP:OD1	1.91	0.69
1:B:183:LEU:O	1:B:187:LEU:HB2	1.92	0.69
1:B:338:VAL:HB	3:B:501:EL3:HAAA	1.74	0.69
1:A:36:HIS:CD2	1:A:61:LYS:H	2.08	0.69
1:A:175:TYR:HB3	1:A:177:ASP:OD1	1.93	0.69
1:A:315:PHE:O	1:A:318:VAL:HG22	1.92	0.69
1:A:176:MET:HG2	1:A:230:ILE:CD1	2.22	0.69
1:A:328:ILE:O	1:A:332:MET:HG3	1.92	0.69
1:B:148:PRO:HA	1:B:458:PRO:O	1.93	0.69
1:B:226:LEU:O	1:B:230:ILE:HG13	1.92	0.69
1:A:140:HIS:O	1:A:143:THR:HB	1.93	0.69
1:B:54:HIS:HB3	1:B:58:VAL:HG11	1.74	0.69
1:A:226:LEU:O	1:A:230:ILE:HG13	1.93	0.69
1:B:281:SER:O	1:B:284:MET:HB2	1.93	0.69
1:A:87:ILE:CD1	1:A:408:ARG:HD2	2.23	0.69
1:B:285:TRP:CH2	1:B:335:ARG:HD2	2.28	0.69
1:A:227:VAL:HG21	1:A:269:VAL:HG22	1.75	0.68
1:A:409:LYS:O	1:A:411:PRO:HD3	1.94	0.68
1:A:86:HIS:C	1:A:87:ILE:HD12	2.18	0.68
1:B:294:PRO:O	1:B:297:ALA:HB3	1.93	0.68
1:A:278:THR:HG22	2:A:500:HEM:HBB2	1.75	0.68
1:A:279:ILE:O	1:A:283:ILE:HG13	1.94	0.68
1:A:333:ARG:HG3	1:A:370:GLN:HB3	1.75	0.68
1:A:174:GLN:HB2	1:A:233:GLU:OE2	1.94	0.68
1:A:79:LEU:CD1	1:A:362:ILE:HD11	2.17	0.68
1:A:187:LEU:HG	1:A:216:PHE:HE2	1.57	0.68
1:B:31:VAL:H	1:B:35:GLY:HA2	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ARG:HA	1:A:394:ASN:HD22	1.59	0.67
1:B:179:ARG:HD3	1:B:226:LEU:HD11	1.74	0.67
1:B:187:LEU:HG	1:B:216:PHE:CE2	2.28	0.67
1:A:49:SER:O	1:A:52:ARG:HB2	1.94	0.67
1:A:90:PRO:CG	1:A:361:ASP:HB3	2.20	0.67
1:A:296:HIS:HD2	1:A:323:HIS:HE1	1.43	0.67
1:A:140:HIS:CE1	1:A:312:PRO:HB3	2.29	0.67
1:A:98:LEU:C	1:A:100:GLY:H	2.00	0.67
1:A:148:PRO:HD3	1:A:431:TYR:OH	1.94	0.67
1:B:33:LEU:HB2	1:B:34:LEU:HD23	1.77	0.67
1:B:431:TYR:CD1	1:B:458:PRO:HB3	2.30	0.67
1:B:113:ARG:O	1:B:116:ARG:HG2	1.95	0.66
1:A:113:ARG:O	1:A:116:ARG:HG2	1.96	0.66
1:A:244:LEU:O	1:A:248:LEU:HB2	1.96	0.66
1:A:87:ILE:HD13	1:A:408:ARG:HD2	1.78	0.66
1:A:87:ILE:HG12	1:A:408:ARG:HD2	1.78	0.66
1:A:96:GLU:HA	1:A:99:LEU:CB	2.26	0.66
1:A:342:THR:O	1:A:343:ARG:HD3	1.94	0.66
1:B:99:LEU:O	1:B:105:ALA:N	2.22	0.66
1:B:146:TRP:HE1	1:B:157:GLU:CG	2.06	0.66
1:B:408:ARG:HH11	1:B:408:ARG:CG	2.07	0.66
1:B:300:ILE:HD11	1:B:327:VAL:HG21	1.77	0.66
1:B:190:VAL:HG21	1:B:216:PHE:CG	2.31	0.66
1:B:75:LEU:O	1:B:79:LEU:HB2	1.96	0.65
1:A:113:ARG:O	1:A:116:ARG:N	2.29	0.65
1:B:87:ILE:N	1:B:87:ILE:CD1	2.56	0.65
1:B:400:MET:HE3	1:B:402:PRO:CG	2.27	0.65
1:A:87:ILE:CG1	1:A:408:ARG:HD2	2.26	0.65
1:A:396:PRO:HB2	1:A:399:ALA:HB2	1.76	0.65
1:B:149:GLY:O	1:B:457:ARG:HD3	1.96	0.65
1:B:87:ILE:HG12	1:B:408:ARG:CD	2.26	0.65
1:B:143:THR:HG23	1:B:430:LYS:HD3	1.77	0.65
1:A:151:THR:HG22	1:A:457:ARG:HG3	1.79	0.65
1:A:190:VAL:HG21	1:A:216:PHE:CG	2.32	0.65
1:A:403:PHE:HD2	1:A:410:CYS:HB3	1.61	0.65
1:B:190:VAL:HG11	1:B:216:PHE:CD1	2.32	0.65
1:A:179:ARG:O	1:A:183:LEU:HG	1.96	0.65
1:A:282:THR:HG21	1:A:420:LEU:HD11	1.77	0.64
1:A:296:HIS:HA	1:A:299:ARG:HB2	1.77	0.64
1:A:333:ARG:HG2	1:A:370:GLN:HB3	1.79	0.64
1:A:48:MET:HE2	1:A:340:VAL:HG13	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:TRP:CZ3	1:B:451:PRO:HG3	2.32	0.64
1:A:234:ARG:CD	1:A:245:LEU:HD22	2.26	0.64
1:A:244:LEU:CD2	1:A:248:LEU:HD12	2.27	0.64
1:A:403:PHE:HB3	1:A:410:CYS:HB3	1.78	0.64
1:A:69:ALA:HA	1:A:363:ILE:O	1.97	0.64
1:A:104:VAL:HG13	1:A:270:ALA:CB	2.28	0.64
1:B:447:ILE:HG22	3:B:501:EL3:HACA	1.79	0.64
1:B:285:TRP:CE3	1:B:335:ARG:HD2	2.33	0.64
1:B:286:LEU:HD21	1:B:328:ILE:HA	1.80	0.64
1:B:48:MET:HE3	1:B:365:SER:HB2	1.79	0.64
1:B:143:THR:HG23	1:B:430:LYS:HD2	1.80	0.63
1:B:378:ASP:HB3	1:B:381:GLU:HB2	1.79	0.63
1:B:226:LEU:HD22	1:B:230:ILE:HD11	1.80	0.63
1:B:317:ASP:O	1:B:320:LYS:N	2.28	0.63
1:B:151:THR:HA	1:B:457:ARG:HG2	1.79	0.63
1:A:239:GLN:C	1:A:241:PRO:HD2	2.24	0.63
1:A:408:ARG:HH11	1:A:408:ARG:CG	2.03	0.63
1:B:100:GLY:HA2	1:B:105:ALA:O	1.98	0.63
1:B:248:LEU:HD11	1:B:267:GLN:HB3	1.81	0.63
1:A:98:LEU:C	1:A:100:GLY:N	2.55	0.63
1:B:224:HIS:ND1	1:B:265:HIS:HE1	1.97	0.62
1:B:86:HIS:HD2	1:B:87:ILE:H	1.46	0.62
1:B:104:VAL:HG13	1:B:270:ALA:CB	2.29	0.62
1:B:385:ASP:O	1:B:391:ARG:NH2	2.32	0.62
1:B:440:ASN:ND2	1:B:452:HIS:CB	2.59	0.62
1:A:142:LEU:CD2	1:A:161:VAL:HG21	2.25	0.62
1:A:388:LEU:HD12	1:A:391:ARG:HH21	1.64	0.62
1:B:31:VAL:N	1:B:35:GLY:HA2	2.14	0.62
1:A:93:GLU:HA	1:A:96:GLU:CB	2.28	0.62
1:A:330:GLU:HA	1:A:330:GLU:OE2	1.98	0.62
1:B:70:VAL:HG21	1:B:362:ILE:HD11	1.81	0.62
1:A:185:VAL:C	1:A:187:LEU:N	2.54	0.62
1:B:171:LEU:HA	1:B:234:ARG:HH12	1.63	0.62
1:A:86:HIS:CD2	1:A:87:ILE:H	2.17	0.62
1:A:120:GLN:O	1:A:124:ARG:HG3	2.00	0.62
1:A:305:GLU:O	1:A:309:GLY:N	2.32	0.62
1:A:403:PHE:CD2	1:A:410:CYS:HB3	2.34	0.62
1:A:355:ARG:O	1:A:357:PRO:HD3	2.00	0.62
1:A:48:MET:CE	1:A:365:SER:HB2	2.30	0.62
1:B:31:VAL:HG12	1:B:32:PRO:CD	2.29	0.61
1:B:350:GLU:HA	1:B:354:TYR:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:HIS:O	1:B:143:THR:HB	2.00	0.61
1:A:274:PRO:CB	3:A:501:EL3:HAHA	2.22	0.61
1:A:185:VAL:O	1:A:187:LEU:N	2.34	0.61
1:B:305:GLU:O	1:B:309:GLY:N	2.32	0.61
1:B:400:MET:HE3	1:B:402:PRO:HG3	1.81	0.61
1:A:339:TRP:HB2	1:A:367:TYR:HB2	1.82	0.61
1:B:239:GLN:C	1:B:241:PRO:HD2	2.25	0.61
1:A:34:LEU:HD23	1:A:34:LEU:N	2.16	0.61
1:A:79:LEU:HD21	1:A:362:ILE:HD13	1.83	0.61
1:A:160:ARG:O	1:A:164:ARG:HG3	2.00	0.61
1:A:244:LEU:HD21	1:A:248:LEU:HD12	1.83	0.61
1:B:318:VAL:HG23	1:B:319:ARG:N	2.16	0.61
1:B:116:ARG:HH11	1:B:267:GLN:NE2	1.98	0.60
1:B:142:LEU:CD2	1:B:161:VAL:HG21	2.16	0.60
1:A:112:HIS:CD2	1:A:113:ARG:N	2.69	0.60
1:B:109:GLY:HA3	1:B:408:ARG:HH22	1.63	0.60
1:B:279:ILE:O	1:B:283:ILE:HG13	2.02	0.60
1:A:318:VAL:HG23	1:A:319:ARG:N	2.16	0.60
1:B:330:GLU:CD	1:B:333:ARG:NH1	2.59	0.60
1:B:330:GLU:OE1	1:B:333:ARG:NH1	2.35	0.60
1:A:95:LEU:O	1:A:99:LEU:N	2.35	0.60
1:A:145:ARG:HH12	1:A:157:GLU:CD	2.10	0.60
1:B:120:GLN:O	1:B:124:ARG:HG3	2.00	0.60
1:A:285:TRP:HE3	1:A:288:GLN:NE2	2.00	0.60
1:A:403:PHE:HB3	1:A:410:CYS:CB	2.32	0.60
1:B:241:PRO:O	1:B:246:THR:HB	2.01	0.60
1:B:403:PHE:CD2	1:B:410:CYS:HB3	2.36	0.60
1:B:403:PHE:HB3	1:B:410:CYS:HB3	1.84	0.60
1:A:31:VAL:HG12	1:A:32:PRO:CD	2.31	0.59
1:A:210:LEU:O	1:A:211:PRO:O	2.20	0.59
1:A:128:ILE:HG12	1:A:129:PRO:HD3	1.81	0.59
1:A:285:TRP:CH2	1:A:451:PRO:HG3	2.36	0.59
1:A:338:VAL:HG23	3:A:501:EL3:HAD	1.83	0.59
1:A:274:PRO:HG2	3:A:501:EL3:HAFA	1.84	0.59
1:B:116:ARG:NH1	1:B:267:GLN:NE2	2.50	0.59
1:A:143:THR:HG23	1:A:430:LYS:HD3	1.84	0.59
1:B:171:LEU:CD2	1:B:245:LEU:HB2	2.33	0.59
1:A:176:MET:HG2	1:A:230:ILE:HD13	1.85	0.59
1:B:308:THR:O	1:B:310:GLY:N	2.36	0.59
1:B:356:ILE:HG22	1:B:356:ILE:O	2.03	0.59
1:A:148:PRO:HG3	1:A:431:TYR:CE2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLY:C	1:A:241:PRO:HD2	2.28	0.59
1:A:440:ASN:ND2	1:A:452:HIS:HB2	2.18	0.58
1:B:404:SER:O	1:B:409:LYS:HG3	2.03	0.58
1:A:60:ILE:HG13	1:A:67:VAL:HG22	1.85	0.58
1:A:403:PHE:HD2	1:A:410:CYS:CB	2.16	0.58
1:B:127:ALA:HB1	1:B:242:ASP:OD2	2.02	0.58
1:B:339:TRP:HB2	1:B:367:TYR:HB2	1.83	0.58
1:A:171:LEU:HA	1:A:234:ARG:HH12	1.68	0.58
1:A:226:LEU:CD2	1:A:230:ILE:HD11	2.34	0.58
1:B:432:ARG:O	1:B:459:VAL:HG13	2.04	0.58
1:A:318:VAL:CG2	1:A:319:ARG:N	2.66	0.58
1:A:444:ARG:HH11	1:A:450:ARG:HD2	1.68	0.58
1:A:149:GLY:O	1:A:457:ARG:HD3	2.03	0.58
1:A:274:PRO:CG	3:A:501:EL3:HAFA	2.33	0.58
1:B:296:HIS:HA	1:B:299:ARG:HB2	1.84	0.58
1:A:29:GLY:H	1:A:36:HIS:HE1	1.51	0.58
1:A:57:VAL:HG23	1:A:57:VAL:O	2.03	0.58
1:B:244:LEU:HD21	1:B:248:LEU:HD12	1.86	0.58
1:A:129:PRO:HG3	1:A:315:PHE:CZ	2.39	0.57
1:B:265:HIS:O	1:B:269:VAL:HG23	2.04	0.57
1:A:36:HIS:HD2	1:A:61:LYS:N	1.96	0.57
1:A:48:MET:HE3	1:A:365:SER:CB	2.34	0.57
1:B:54:HIS:CB	1:B:58:VAL:HG11	2.33	0.57
1:B:95:LEU:O	1:B:99:LEU:N	2.37	0.57
1:A:333:ARG:HA	1:A:370:GLN:NE2	2.19	0.57
1:A:427:LEU:HD22	1:A:433:PHE:HZ	1.70	0.57
1:B:412:SER:O	1:B:416:SER:N	2.36	0.57
1:A:176:MET:HG2	1:A:230:ILE:HD11	1.86	0.57
1:B:161:VAL:O	1:B:165:VAL:HG23	2.05	0.57
1:B:366:PRO:O	1:B:370:GLN:HG3	2.05	0.57
1:A:350:GLU:HA	1:A:354:TYR:O	2.04	0.57
1:A:373:PRO:HG3	1:A:379:ASN:ND2	2.20	0.57
1:A:185:VAL:C	1:A:187:LEU:H	2.12	0.56
1:B:93:GLU:HA	1:B:96:GLU:CB	2.34	0.56
1:A:403:PHE:N	1:A:403:PHE:CD1	2.73	0.56
1:A:221:ALA:O	1:A:225:LEU:HB2	2.06	0.56
1:A:234:ARG:HH11	1:A:245:LEU:HB3	1.71	0.56
1:A:339:TRP:CD2	1:A:340:VAL:HG22	2.40	0.56
1:B:154:ALA:O	1:B:158:SER:HB2	2.05	0.56
1:B:245:LEU:HD23	1:B:245:LEU:C	2.29	0.56
1:B:98:LEU:O	1:B:102:GLU:N	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:THR:HG21	1:A:436:VAL:HG21	1.86	0.56
2:B:500:HEM:C1A	3:B:501:EL3:HAE	2.40	0.56
1:A:279:ILE:HD13	2:A:500:HEM:CMC	2.35	0.56
1:B:318:VAL:CG2	1:B:319:ARG:N	2.67	0.56
1:A:400:MET:HE3	1:A:402:PRO:CG	2.35	0.56
1:B:391:ARG:HA	1:B:394:ASN:ND2	2.14	0.56
1:A:408:ARG:HA	2:A:500:HEM:O2D	2.06	0.56
1:A:412:SER:HB3	1:A:415:PHE:HB3	1.88	0.56
1:B:244:LEU:CD2	1:B:248:LEU:HD12	2.36	0.56
1:A:87:ILE:HD12	1:A:87:ILE:H	1.66	0.56
1:B:87:ILE:CD1	1:B:408:ARG:HD2	2.36	0.56
1:B:440:ASN:HD21	1:B:452:HIS:HB2	1.67	0.56
1:A:222:ASP:O	1:A:226:LEU:HB2	2.06	0.55
1:B:388:LEU:O	1:B:389:PRO:C	2.50	0.55
1:A:151:THR:CG2	1:A:436:VAL:HG21	2.36	0.55
1:B:90:PRO:HG3	1:B:361:ASP:CG	2.31	0.55
1:B:174:GLN:HG3	1:B:233:GLU:CD	2.31	0.55
1:B:36:HIS:CD2	1:B:61:LYS:H	2.19	0.55
1:B:99:LEU:HA	1:B:103:GLY:H	1.72	0.55
1:B:291:ALA:HA	1:B:433:PHE:O	2.07	0.55
1:A:22:ARG:HH11	1:A:355:ARG:HD2	1.72	0.55
1:A:227:VAL:HG21	1:A:269:VAL:CG2	2.36	0.55
1:B:49:SER:O	1:B:52:ARG:HB2	2.06	0.55
1:B:279:ILE:HD13	2:B:500:HEM:HMC1	1.88	0.55
1:B:51:LEU:HG	1:B:58:VAL:HG21	1.87	0.55
1:A:82:ASN:OD1	1:A:84:ASP:HB2	2.07	0.55
1:A:348:GLU:CA	1:A:358:ALA:HB2	2.36	0.54
1:A:33:LEU:HB2	1:A:34:LEU:CD2	2.35	0.54
1:A:403:PHE:HD2	1:A:410:CYS:SG	2.29	0.54
1:B:138:GLU:OE1	1:B:164:ARG:NH1	2.36	0.54
1:A:92:TRP:HE1	3:A:501:EL3:HAI	1.72	0.54
1:A:337:ALA:O	1:A:448:THR:HA	2.08	0.54
1:B:142:LEU:HD11	1:B:161:VAL:CG2	2.28	0.54
1:B:296:HIS:O	1:B:300:ILE:N	2.40	0.54
1:A:114:ARG:C	1:A:116:ARG:N	2.63	0.54
1:B:329:VAL:HG13	1:B:400:MET:HE2	1.88	0.54
1:A:104:VAL:O	1:A:105:ALA:CB	2.55	0.54
1:B:92:TRP:CZ2	3:B:501:EL3:CAB	2.74	0.54
1:B:143:THR:CG2	1:B:430:LYS:HD2	2.37	0.54
1:B:86:HIS:C	1:B:87:ILE:HD12	2.33	0.54
1:B:90:PRO:CD	1:B:361:ASP:OD2	2.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ARG:NH1	1:B:267:GLN:HE21	2.05	0.54
1:A:104:VAL:O	1:A:105:ALA:HB3	2.07	0.54
1:A:413:ASP:OD2	1:A:414:HIS:N	2.40	0.54
1:B:160:ARG:HG3	1:B:181:GLU:CD	2.33	0.54
1:B:343:ARG:HB2	1:B:362:ILE:HG23	1.89	0.54
1:B:444:ARG:HH11	1:B:450:ARG:HD2	1.73	0.54
1:A:164:ARG:O	1:A:168:ARG:HB2	2.08	0.54
1:A:190:VAL:HG21	1:A:216:PHE:HB2	1.90	0.54
1:A:263:GLU:HG2	1:A:263:GLU:O	2.07	0.54
1:A:435:GLN:HE21	1:A:439:SER:CB	2.18	0.54
1:B:81:LEU:HG	1:B:405:ALA:HB3	1.89	0.54
1:A:40:LEU:O	1:A:44:PRO:HG3	2.08	0.53
1:B:161:VAL:HG11	1:B:423:ILE:CD1	2.38	0.53
1:B:275:GLY:HA3	2:B:500:HEM:HBC2	1.90	0.53
1:A:48:MET:HE2	1:A:340:VAL:CG1	2.37	0.53
1:B:339:TRP:CD2	1:B:340:VAL:HG22	2.44	0.53
1:A:226:LEU:HD23	1:A:230:ILE:HD11	1.89	0.53
1:B:326:ASN:HB3	1:B:384:PRO:O	2.09	0.53
1:A:118:THR:O	1:A:121:PRO:HD2	2.08	0.53
1:B:171:LEU:HD22	1:B:245:LEU:HD12	1.88	0.53
1:A:322:ARG:O	1:A:326:ASN:ND2	2.37	0.53
1:A:138:GLU:OE1	1:A:164:ARG:NH1	2.42	0.53
1:A:282:THR:HG21	1:A:420:LEU:CD1	2.39	0.53
1:A:286:LEU:HD21	1:A:328:ILE:HA	1.92	0.53
1:A:432:ARG:HB3	1:A:459:VAL:CG2	2.38	0.53
1:B:33:LEU:C	1:B:34:LEU:HD23	2.33	0.53
1:B:445:VAL:HA	1:B:449:LEU:HD23	1.90	0.53
1:A:100:GLY:HA2	1:A:105:ALA:C	2.34	0.52
1:B:301:ARG:O	1:B:301:ARG:HG2	2.10	0.52
1:B:444:ARG:NH1	1:B:450:ARG:HD2	2.25	0.52
1:A:33:LEU:C	1:A:34:LEU:HD23	2.35	0.52
1:A:75:LEU:O	1:A:79:LEU:HB2	2.10	0.52
1:A:114:ARG:O	1:A:116:ARG:N	2.42	0.52
1:B:227:VAL:HG21	1:B:269:VAL:HG22	1.90	0.52
1:A:216:PHE:CD2	1:A:216:PHE:O	2.63	0.52
1:A:274:PRO:CB	3:A:501:EL3:HAFA	2.40	0.52
1:B:113:ARG:O	1:B:114:ARG:C	2.53	0.52
1:A:225:LEU:HD23	1:A:229:GLU:OE2	2.10	0.52
1:A:238:GLY:O	1:A:241:PRO:HD2	2.09	0.52
1:A:22:ARG:HH11	1:A:355:ARG:CD	2.23	0.52
1:B:86:HIS:CD2	1:B:87:ILE:H	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:PHE:HE1	1:B:458:PRO:HG3	1.75	0.52
1:A:87:ILE:HG12	1:A:408:ARG:CD	2.39	0.52
1:A:113:ARG:O	1:A:114:ARG:C	2.53	0.52
1:B:81:LEU:HD21	1:B:405:ALA:CB	2.37	0.52
1:B:113:ARG:O	1:B:115:GLN:N	2.42	0.52
1:B:234:ARG:HD2	1:B:245:LEU:HD22	1.92	0.52
1:A:240:LYS:O	1:A:240:LYS:HG2	2.10	0.52
1:B:69:ALA:HA	1:B:363:ILE:O	2.10	0.52
1:B:378:ASP:HB3	1:B:381:GLU:CB	2.40	0.52
1:A:285:TRP:CE3	1:A:288:GLN:NE2	2.78	0.52
1:B:173:GLY:O	1:B:175:TYR:CE2	2.63	0.52
1:A:108:ASN:O	1:A:109:GLY:C	2.53	0.51
1:B:104:VAL:O	1:B:105:ALA:CB	2.57	0.51
1:B:139:ALA:C	1:B:141:ALA:N	2.68	0.51
1:A:135:MET:SD	1:A:419:GLN:HB3	2.49	0.51
1:A:265:HIS:O	1:A:265:HIS:ND1	2.43	0.51
1:A:301:ARG:HH11	1:A:301:ARG:CB	2.09	0.51
1:B:427:LEU:HD22	1:B:433:PHE:HZ	1.75	0.51
1:A:400:MET:HE3	1:A:402:PRO:HD3	1.92	0.51
1:B:104:VAL:O	1:B:105:ALA:HB3	2.10	0.51
1:B:240:LYS:O	1:B:242:ASP:N	2.44	0.51
1:A:244:LEU:C	1:A:244:LEU:HD23	2.36	0.51
1:B:240:LYS:N	1:B:241:PRO:CD	2.74	0.51
1:A:318:VAL:C	1:A:320:LYS:H	2.18	0.51
1:B:25:PRO:O	1:B:59:ARG:NH2	2.43	0.51
1:A:419:GLN:O	1:A:423:ILE:HG13	2.11	0.51
1:B:318:VAL:C	1:B:320:LYS:H	2.19	0.51
1:A:60:ILE:CG1	1:A:67:VAL:HG22	2.41	0.51
1:B:151:THR:CG2	1:B:436:VAL:HG21	2.41	0.51
1:B:445:VAL:O	1:B:445:VAL:HG13	2.10	0.51
1:A:90:PRO:HD3	1:A:361:ASP:OD2	2.11	0.50
2:B:500:HEM:CHA	3:B:501:EL3:HAF	2.41	0.50
1:A:146:TRP:CE2	1:A:152:VAL:HG11	2.45	0.50
1:B:145:ARG:HH21	1:B:160:ARG:NH1	2.09	0.50
1:B:106:THR:O	1:B:107:ALA:HB3	2.11	0.50
1:A:378:ASP:HB3	1:A:381:GLU:HB2	1.92	0.50
1:B:161:VAL:HG11	1:B:423:ILE:HD13	1.93	0.50
1:B:275:GLY:HA3	2:B:500:HEM:CBC	2.41	0.50
1:A:244:LEU:O	1:A:244:LEU:HD23	2.12	0.50
1:B:25:PRO:HG2	1:B:68:TYR:HD2	1.77	0.50
1:B:192:ARG:NH1	1:B:277:GLU:OE2	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:GLU:CA	1:B:358:ALA:HB2	2.41	0.50
1:B:216:PHE:O	1:B:216:PHE:CD2	2.64	0.50
1:A:115:GLN:O	1:A:116:ARG:HD3	2.12	0.50
1:B:87:ILE:HD11	1:B:408:ARG:HG3	1.94	0.50
1:B:226:LEU:CD2	1:B:230:ILE:HD11	2.42	0.50
1:B:338:VAL:HG11	2:B:500:HEM:HMA2	1.94	0.50
1:A:179:ARG:HG2	1:A:226:LEU:CD1	2.41	0.49
1:A:304:VAL:O	1:A:308:THR:HG22	2.11	0.49
1:A:427:LEU:HD22	1:A:433:PHE:CZ	2.46	0.49
1:B:109:GLY:O	1:B:110:PRO:O	2.30	0.49
1:B:212:ALA:HB3	1:B:216:PHE:CD1	2.42	0.49
1:B:430:LYS:HG2	1:B:431:TYR:CE2	2.47	0.49
1:A:105:ALA:HB3	1:A:266:ASP:HB3	1.94	0.49
1:A:151:THR:CG2	1:A:457:ARG:NH1	2.76	0.49
1:A:343:ARG:HB2	1:A:362:ILE:HG23	1.94	0.49
1:A:81:LEU:CD2	1:A:405:ALA:HB1	2.41	0.49
1:A:134:ILE:HG21	1:A:168:ARG:HB3	1.94	0.49
1:A:240:LYS:O	1:A:242:ASP:N	2.45	0.49
1:B:279:ILE:O	1:B:279:ILE:HG23	2.12	0.49
1:A:158:SER:OG	1:A:283:ILE:CG2	2.60	0.49
1:B:225:LEU:HD23	1:B:229:GLU:OE2	2.11	0.49
1:A:118:THR:HG21	1:A:251:ALA:HB2	1.93	0.49
1:B:31:VAL:O	1:B:35:GLY:HA2	2.12	0.49
1:A:296:HIS:CD2	1:A:323:HIS:CE1	2.95	0.49
1:A:388:LEU:O	1:A:389:PRO:C	2.56	0.49
1:B:171:LEU:HD22	1:B:245:LEU:HB2	1.94	0.49
1:B:238:GLY:C	1:B:241:PRO:HD2	2.38	0.49
1:A:182:ARG:O	1:A:185:VAL:HB	2.12	0.49
1:A:341:LEU:HB2	1:A:364:TYR:CE2	2.47	0.49
1:A:160:ARG:C	1:A:162:ALA:N	2.69	0.48
1:A:88:ALA:O	1:A:89:GLY:C	2.56	0.48
1:A:142:LEU:O	1:A:145:ARG:N	2.46	0.48
1:A:179:ARG:CG	1:A:226:LEU:HD11	2.44	0.48
1:A:356:ILE:O	1:A:356:ILE:HG22	2.13	0.48
1:B:105:ALA:CB	1:B:266:ASP:CG	2.86	0.48
1:B:285:TRP:CH2	1:B:451:PRO:HG3	2.48	0.48
1:B:348:GLU:H	1:B:358:ALA:HB2	1.75	0.48
1:A:113:ARG:O	1:A:115:GLN:N	2.46	0.48
1:A:151:THR:HG23	1:A:457:ARG:NH1	2.28	0.48
1:A:240:LYS:N	1:A:241:PRO:CD	2.77	0.48
1:B:373:PRO:HG3	1:B:379:ASN:ND2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ALA:O	1:A:163:VAL:C	2.55	0.48
1:A:174:GLN:HG3	1:A:233:GLU:CD	2.38	0.48
1:A:185:VAL:O	1:A:186:ALA:C	2.57	0.48
1:B:87:ILE:HD12	1:B:87:ILE:H	1.70	0.48
1:B:301:ARG:HH11	1:B:301:ARG:HB3	1.78	0.48
1:B:349:SER:O	1:B:356:ILE:N	2.45	0.48
1:A:280:ALA:O	1:A:281:SER:C	2.57	0.48
1:A:295:GLU:HG2	1:A:296:HIS:H	1.78	0.48
1:A:305:GLU:HA	1:A:308:THR:HG22	1.94	0.48
1:A:68:TYR:O	1:A:362:ILE:HA	2.14	0.48
1:A:317:ASP:O	1:A:320:LYS:N	2.36	0.48
1:A:317:ASP:O	1:A:320:LYS:HB2	2.14	0.48
1:B:36:HIS:HD2	1:B:61:LYS:N	2.06	0.48
1:A:145:ARG:NH2	1:A:160:ARG:NH1	2.62	0.48
1:A:333:ARG:HD2	1:A:376:TYR:CZ	2.49	0.48
1:A:341:LEU:HD12	1:A:364:TYR:CZ	2.49	0.48
1:A:402:PRO:HB2	1:A:403:PHE:CD1	2.49	0.48
1:B:98:LEU:C	1:B:100:GLY:H	2.21	0.47
1:B:139:ALA:O	1:B:142:LEU:N	2.46	0.47
1:B:310:GLY:O	1:B:311:ARG:C	2.57	0.47
1:B:448:THR:HG22	3:B:501:EL3:HAC	1.95	0.47
1:A:61:LYS:HG2	1:A:66:THR:HG22	1.91	0.47
1:A:135:MET:HE1	1:A:418:ALA:CB	2.42	0.47
1:A:127:ALA:HB1	1:A:242:ASP:OD2	2.14	0.47
1:A:174:GLN:HG3	1:A:233:GLU:OE2	2.15	0.47
1:B:108:ASN:O	1:B:109:GLY:C	2.57	0.47
1:B:240:LYS:O	1:B:240:LYS:HG2	2.14	0.47
1:A:388:LEU:HD12	1:A:391:ARG:NH2	2.29	0.47
1:A:154:ALA:O	1:A:158:SER:HB2	2.15	0.47
1:A:176:MET:O	1:A:177:ASP:C	2.57	0.47
1:A:241:PRO:O	1:A:246:THR:HB	2.14	0.47
1:B:31:VAL:CG1	1:B:32:PRO:HD2	2.39	0.47
1:B:447:ILE:O	3:B:501:EL3:HACA	2.14	0.47
1:A:36:HIS:O	1:A:38:TRP:N	2.47	0.47
1:A:89:GLY:HA2	1:A:90:PRO:HD2	1.58	0.47
1:A:105:ALA:CB	1:A:266:ASP:CG	2.88	0.47
1:A:143:THR:HG23	1:A:430:LYS:CD	2.45	0.47
1:A:330:GLU:OE1	1:A:333:ARG:NH1	2.47	0.47
1:B:31:VAL:H	1:B:35:GLY:CA	2.27	0.47
1:B:92:TRP:CE2	3:B:501:EL3:HABB	2.45	0.47
1:B:224:HIS:ND1	1:B:265:HIS:CE1	2.81	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:MET:HE3	1:A:402:PRO:CD	2.45	0.47
1:B:338:VAL:HG23	3:B:501:EL3:HAD	1.97	0.47
1:B:436:VAL:HG12	1:B:437:ALA:O	2.15	0.47
1:A:31:VAL:CG1	1:A:32:PRO:HD2	2.42	0.47
1:A:125:LEU:HD12	1:A:125:LEU:H	1.78	0.47
1:B:347:ALA:O	1:B:348:GLU:C	2.58	0.47
1:B:348:GLU:HA	1:B:358:ALA:N	2.29	0.47
1:A:439:SER:HA	1:A:455:LEU:HD12	1.97	0.47
1:B:176:MET:HG2	1:B:230:ILE:HD13	1.97	0.47
1:B:179:ARG:CD	1:B:226:LEU:HD11	2.44	0.47
1:B:210:LEU:O	1:B:211:PRO:O	2.32	0.47
1:A:348:GLU:HA	1:A:358:ALA:N	2.29	0.46
1:B:117:ARG:O	1:B:121:PRO:HD3	2.16	0.46
1:B:145:ARG:NE	1:B:160:ARG:NH2	2.62	0.46
1:B:171:LEU:HD23	1:B:245:LEU:HB2	1.97	0.46
1:A:179:ARG:HG2	1:A:226:LEU:HD11	1.97	0.46
1:A:234:ARG:NH1	1:A:243:ASP:OD2	2.48	0.46
1:B:317:ASP:O	1:B:320:LYS:HB2	2.15	0.46
1:B:326:ASN:OD1	1:B:387:TRP:HB2	2.15	0.46
1:B:403:PHE:CZ	1:B:413:ASP:HA	2.45	0.46
1:B:433:PHE:CE1	1:B:458:PRO:HG3	2.49	0.46
1:B:89:GLY:HA2	1:B:90:PRO:HD2	1.58	0.46
1:B:114:ARG:O	1:B:116:ARG:N	2.47	0.46
1:B:185:VAL:C	1:B:187:LEU:H	2.22	0.46
1:B:310:GLY:O	1:B:311:ARG:O	2.33	0.46
1:A:349:SER:OG	1:A:350:GLU:N	2.47	0.46
1:A:160:ARG:HG3	1:A:181:GLU:CD	2.41	0.46
1:A:240:LYS:O	1:A:241:PRO:C	2.55	0.46
1:A:245:LEU:HD23	1:A:245:LEU:C	2.40	0.46
1:B:70:VAL:CG2	1:B:362:ILE:HD11	2.44	0.46
1:A:244:LEU:HD11	1:A:271:ILE:HD13	1.93	0.46
1:A:339:TRP:H	1:A:339:TRP:CD1	2.33	0.46
1:B:44:PRO:HG2	1:B:445:VAL:HG11	1.97	0.46
1:B:136:GLU:HG2	1:B:314:ALA:HA	1.98	0.46
1:B:444:ARG:HB3	1:B:450:ARG:O	2.15	0.46
1:A:248:LEU:HD22	1:A:264:ILE:HG23	1.96	0.46
1:B:185:VAL:C	1:B:187:LEU:N	2.74	0.46
1:B:403:PHE:HD2	1:B:410:CYS:CB	2.27	0.46
1:A:36:HIS:C	1:A:38:TRP:N	2.74	0.46
1:A:141:ALA:O	1:A:142:LEU:C	2.59	0.46
1:B:38:TRP:CD1	1:B:38:TRP:C	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:GLN:O	1:B:176:MET:HE2	2.16	0.46
1:A:301:ARG:HD2	1:A:429:THR:O	2.16	0.46
1:B:234:ARG:HD3	1:B:246:THR:OG1	2.15	0.46
1:B:90:PRO:O	1:B:91:LEU:HD23	2.15	0.46
1:B:334:LEU:HD12	1:B:382:PHE:HD1	1.81	0.46
1:A:397:LYS:HE3	1:B:395:VAL:O	2.16	0.45
1:B:176:MET:O	1:B:177:ASP:C	2.59	0.45
1:A:57:VAL:O	1:A:57:VAL:CG2	2.63	0.45
1:A:293:HIS:O	1:A:294:PRO:C	2.59	0.45
1:A:397:LYS:HA	1:B:397:LYS:CE	2.46	0.45
1:B:139:ALA:O	1:B:141:ALA:N	2.49	0.45
1:B:217:ASN:C	1:B:219:ALA:H	2.23	0.45
1:B:385:ASP:O	1:B:391:ARG:CZ	2.65	0.45
1:A:140:HIS:NE2	1:A:312:PRO:HB3	2.31	0.45
1:A:178:GLU:HA	1:A:181:GLU:CD	2.40	0.45
1:B:68:TYR:OH	1:B:357:PRO:HG2	2.16	0.45
1:B:238:GLY:O	1:B:241:PRO:HD2	2.16	0.45
1:B:241:PRO:HB2	1:B:246:THR:OG1	2.16	0.45
1:B:430:LYS:HE2	1:B:431:TYR:OH	2.17	0.45
1:A:106:THR:O	1:A:107:ALA:HB3	2.17	0.45
1:A:111:LEU:O	1:A:112:HIS:CG	2.69	0.45
1:A:378:ASP:HB3	1:A:381:GLU:CB	2.46	0.45
1:A:397:LYS:HE3	1:B:396:PRO:O	2.16	0.45
1:B:262:GLN:O	1:B:262:GLN:HG2	2.17	0.45
1:A:444:ARG:NH1	1:A:450:ARG:HD2	2.32	0.45
1:B:406:GLY:O	1:B:409:LYS:HB2	2.16	0.45
1:A:318:VAL:C	1:A:320:LYS:N	2.75	0.45
1:B:170:LEU:O	1:B:171:LEU:CD2	2.55	0.45
1:B:90:PRO:CG	1:B:361:ASP:OD2	2.65	0.45
1:B:115:GLN:O	1:B:116:ARG:HD3	2.17	0.45
1:A:49:SER:HB3	1:A:52:ARG:HH22	1.78	0.45
1:B:90:PRO:CD	1:B:361:ASP:HB3	2.46	0.45
1:B:98:LEU:C	1:B:100:GLY:N	2.74	0.45
1:B:174:GLN:HB2	1:B:233:GLU:OE2	2.16	0.45
1:B:287:LEU:O	1:B:288:GLN:C	2.58	0.45
1:A:120:GLN:HB2	1:A:121:PRO:HD3	1.98	0.45
1:B:240:LYS:O	1:B:241:PRO:C	2.56	0.45
1:A:52:ARG:NH1	1:A:368:ALA:HB1	2.28	0.44
1:B:36:HIS:CD2	1:B:60:ILE:HB	2.52	0.44
1:B:304:VAL:O	1:B:308:THR:HB	2.17	0.44
1:B:318:VAL:C	1:B:320:LYS:N	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:LYS:HE2	1:B:431:TYR:CE2	2.53	0.44
2:B:500:HEM:HMA1	2:B:500:HEM:HBA1	1.99	0.44
1:B:114:ARG:C	1:B:116:ARG:N	2.62	0.44
1:B:440:ASN:HD21	1:B:452:HIS:CB	2.29	0.44
1:A:111:LEU:C	1:A:113:ARG:N	2.76	0.44
1:B:132:GLY:O	1:B:136:GLU:HG3	2.17	0.44
1:B:146:TRP:CE2	1:B:152:VAL:HG11	2.52	0.44
1:B:300:ILE:O	1:B:300:ILE:HG22	2.16	0.44
1:B:317:ASP:O	1:B:318:VAL:C	2.60	0.44
1:A:24:PRO:HA	1:A:25:PRO:HD3	1.88	0.44
1:A:33:LEU:CB	1:A:34:LEU:HD23	2.44	0.44
1:A:90:PRO:HG3	1:A:361:ASP:CG	2.43	0.44
1:A:151:THR:HG22	1:A:457:ARG:CZ	2.48	0.44
1:A:190:VAL:HG21	1:A:216:PHE:CB	2.46	0.44
1:A:445:VAL:HA	1:A:449:LEU:HD23	1.99	0.44
1:A:45:LEU:HD21	1:A:449:LEU:HD21	1.99	0.44
1:A:153:ASP:O	1:A:157:GLU:HB2	2.18	0.44
1:A:176:MET:O	1:A:177:ASP:O	2.35	0.44
1:A:300:ILE:HG22	1:A:300:ILE:O	2.17	0.44
1:A:317:ASP:O	1:A:318:VAL:C	2.60	0.44
1:B:112:HIS:C	1:B:114:ARG:N	2.74	0.44
1:B:427:LEU:HD22	1:B:433:PHE:CZ	2.52	0.44
1:A:111:LEU:HD22	1:A:111:LEU:HA	1.63	0.44
1:A:112:HIS:C	1:A:114:ARG:N	2.75	0.44
1:A:191:PHE:CD1	1:A:447:ILE:HD11	2.53	0.44
1:A:239:GLN:C	1:A:241:PRO:CD	2.91	0.44
1:A:262:GLN:O	1:A:262:GLN:HG2	2.17	0.44
1:B:29:GLY:N	1:B:36:HIS:CE1	2.60	0.44
1:A:172:ARG:HB2	1:A:234:ARG:NH2	2.32	0.44
1:B:183:LEU:HD22	1:B:222:ASP:HB3	1.99	0.44
1:A:77:GLY:O	1:A:78:ALA:C	2.60	0.44
1:A:339:TRP:CE3	1:A:340:VAL:HG22	2.53	0.44
1:A:385:ASP:O	1:A:391:ARG:NH2	2.51	0.44
1:A:90:PRO:CG	1:A:361:ASP:OD2	2.66	0.44
1:A:146:TRP:CZ2	1:A:152:VAL:HG11	2.53	0.44
1:B:51:LEU:HG	1:B:58:VAL:CG2	2.48	0.44
1:B:111:LEU:HA	1:B:111:LEU:HD22	1.64	0.44
1:B:435:GLN:HE21	1:B:439:SER:HB3	1.83	0.44
3:B:501:EL3:HACB	3:B:501:EL3:HAGA	1.84	0.44
1:A:401:LYS:O	1:A:403:PHE:O	2.36	0.43
1:B:137:GLU:O	1:B:141:ALA:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:CG2	1:A:251:ALA:HB2	2.48	0.43
1:B:336:PRO:O	1:B:337:ALA:C	2.61	0.43
1:A:29:GLY:N	1:A:36:HIS:HE1	2.15	0.43
1:A:165:VAL:HG11	1:A:419:GLN:CD	2.43	0.43
1:A:333:ARG:NH2	1:A:379:ASN:O	2.52	0.43
1:B:229:GLU:O	1:B:232:ALA:HB3	2.19	0.43
1:A:275:GLY:HA3	2:A:500:HEM:C3C	2.54	0.43
1:A:348:GLU:H	1:A:358:ALA:HB2	1.76	0.43
1:A:358:ALA:C	1:A:360:ALA:H	2.25	0.43
1:B:112:HIS:HD2	1:B:113:ARG:C	2.26	0.43
1:B:330:GLU:CD	1:B:333:ARG:HH12	2.23	0.43
1:B:334:LEU:HD11	1:B:382:PHE:HA	2.00	0.43
1:A:140:HIS:NE2	1:A:312:PRO:CB	2.82	0.43
1:B:112:HIS:CG	1:B:113:ARG:N	2.86	0.43
1:A:90:PRO:HG3	1:A:361:ASP:OD2	2.18	0.43
1:A:116:ARG:HH11	1:A:267:GLN:NE2	2.16	0.43
1:B:111:LEU:C	1:B:113:ARG:N	2.76	0.43
1:B:113:ARG:O	1:B:116:ARG:CG	2.64	0.43
1:B:123:PHE:HB3	1:B:411:PRO:O	2.19	0.43
1:A:34:LEU:O	1:A:35:GLY:C	2.62	0.43
1:A:40:LEU:HD22	1:A:62:LEU:HD21	2.01	0.43
1:A:86:HIS:CD2	1:A:87:ILE:N	2.84	0.43
1:A:287:LEU:HA	1:A:287:LEU:HD23	1.71	0.43
1:A:342:THR:HG23	1:A:362:ILE:O	2.19	0.43
1:A:404:SER:O	1:A:409:LYS:HG3	2.18	0.43
1:B:179:ARG:NH1	1:B:226:LEU:HG	2.34	0.43
1:B:244:LEU:CD1	1:B:271:ILE:HD13	2.35	0.43
1:B:296:HIS:HD2	1:B:323:HIS:CE1	2.37	0.43
1:A:136:GLU:HG2	1:A:314:ALA:HA	2.00	0.43
1:A:288:GLN:HE21	1:A:288:GLN:HB3	1.55	0.43
1:A:291:ALA:HA	1:A:433:PHE:O	2.19	0.43
1:A:314:ALA:O	1:A:315:PHE:C	2.61	0.43
1:B:159:PHE:O	1:B:163:VAL:HG23	2.19	0.43
1:B:159:PHE:HE2	1:B:184:CYS:HB2	1.84	0.43
1:B:176:MET:HG2	1:B:230:ILE:CD1	2.49	0.43
1:B:324:THR:O	1:B:328:ILE:HG13	2.18	0.43
1:B:412:SER:O	1:B:413:ASP:C	2.62	0.43
1:B:25:PRO:HG2	1:B:68:TYR:CD2	2.53	0.43
1:B:27:ALA:HA	1:B:59:ARG:O	2.19	0.43
1:B:192:ARG:HH12	1:B:277:GLU:CD	2.23	0.43
1:B:220:LEU:O	1:B:223:LEU:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ARG:NH1	1:A:355:ARG:HE	2.17	0.42
1:A:38:TRP:O	1:A:39:ARG:C	2.60	0.42
1:A:99:LEU:O	1:A:105:ALA:N	2.45	0.42
1:B:315:PHE:CD2	1:B:315:PHE:C	2.96	0.42
1:A:86:HIS:CA	1:A:87:ILE:HD12	2.49	0.42
1:A:212:ALA:HB1	1:A:213:ASN:H	1.70	0.42
1:B:230:ILE:HA	1:B:233:GLU:HG2	2.01	0.42
1:A:75:LEU:HD21	1:A:352:GLY:HA3	2.01	0.42
1:A:89:GLY:O	1:A:92:TRP:HB3	2.17	0.42
1:B:47:PHE:CZ	1:B:51:LEU:HD13	2.54	0.42
1:B:50:GLN:O	1:B:51:LEU:C	2.62	0.42
1:B:145:ARG:HH12	1:B:157:GLU:CD	2.27	0.42
1:B:181:GLU:O	1:B:185:VAL:HG23	2.19	0.42
1:B:212:ALA:HB1	1:B:213:ASN:H	1.69	0.42
1:A:22:ARG:HD3	1:A:355:ARG:HD2	2.01	0.42
1:A:125:LEU:HG	1:A:414:HIS:CE1	2.55	0.42
1:A:430:LYS:HE2	1:A:431:TYR:CZ	2.55	0.42
1:A:123:PHE:CE2	1:A:412:SER:OG	2.71	0.42
1:B:128:ILE:HG12	1:B:129:PRO:HD3	1.94	0.42
1:A:432:ARG:CB	1:A:459:VAL:HG22	2.44	0.42
1:B:48:MET:HE3	1:B:365:SER:CB	2.45	0.42
1:B:333:ARG:HD2	1:B:376:TYR:CZ	2.54	0.42
1:A:74:GLU:H	1:A:74:GLU:HG3	1.63	0.42
1:A:131:TYR:HB3	1:A:169:CYS:SG	2.59	0.42
1:B:34:LEU:HD23	1:B:34:LEU:N	2.35	0.42
1:B:111:LEU:HB3	1:B:112:HIS:H	1.63	0.42
1:B:215:ARG:C	1:B:217:ASN:N	2.77	0.42
1:B:267:GLN:O	1:B:271:ILE:HD12	2.20	0.42
1:A:135:MET:HE3	1:A:422:LEU:HD12	2.02	0.42
1:B:89:GLY:O	1:B:92:TRP:HB3	2.19	0.42
1:B:128:ILE:HA	1:B:131:TYR:CD1	2.55	0.42
1:B:190:VAL:HG21	1:B:216:PHE:HB2	2.01	0.42
1:B:221:ALA:O	1:B:225:LEU:HB2	2.20	0.42
1:B:430:LYS:HG2	1:B:431:TYR:CD2	2.54	0.42
1:A:285:TRP:CH2	1:A:335:ARG:HD2	2.55	0.41
1:A:72:ASN:O	1:A:73:PRO:C	2.62	0.41
1:A:85:TYR:HB3	1:A:343:ARG:HB3	2.03	0.41
1:A:134:ILE:HD11	1:A:172:ARG:HE	1.85	0.41
1:B:430:LYS:HE2	1:B:431:TYR:CZ	2.55	0.41
1:A:151:THR:CG2	1:A:457:ARG:CZ	2.98	0.41
1:A:238:GLY:O	1:A:239:GLN:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:LEU:HD23	1:A:286:LEU:HA	1.95	0.41
1:A:402:PRO:HB2	1:A:403:PHE:CE1	2.56	0.41
1:B:296:HIS:O	1:B:297:ALA:C	2.62	0.41
1:A:357:PRO:O	1:A:360:ALA:HB2	2.21	0.41
1:B:244:LEU:HD23	1:B:244:LEU:C	2.45	0.41
1:B:244:LEU:O	1:B:248:LEU:HB2	2.20	0.41
1:B:288:GLN:HE21	1:B:288:GLN:HB3	1.51	0.41
1:B:304:VAL:HG13	1:B:313:VAL:HG22	2.02	0.41
1:A:31:VAL:O	1:A:35:GLY:HA2	2.20	0.41
1:B:285:TRP:CZ2	1:B:335:ARG:HD2	2.55	0.41
1:A:36:HIS:O	1:A:37:GLY:C	2.63	0.41
1:B:431:TYR:HB3	1:B:432:ARG:H	1.62	0.41
1:A:142:LEU:CD1	1:A:161:VAL:CG2	2.89	0.41
1:A:397:LYS:HA	1:B:397:LYS:HE3	2.03	0.41
1:A:431:TYR:HB3	1:A:432:ARG:H	1.54	0.41
1:A:70:VAL:HG21	1:A:362:ILE:HD11	2.03	0.41
1:A:113:ARG:O	1:A:116:ARG:CG	2.68	0.41
1:A:117:ARG:O	1:A:117:ARG:HG2	2.21	0.41
1:A:185:VAL:HG12	1:A:186:ALA:N	2.36	0.41
1:B:36:HIS:C	1:B:38:TRP:N	2.79	0.41
1:B:120:GLN:N	1:B:121:PRO:CD	2.84	0.41
1:B:153:ASP:O	1:B:157:GLU:HB2	2.21	0.41
1:B:410:CYS:HA	1:B:411:PRO:HD3	1.90	0.41
1:A:81:LEU:HD11	1:A:398:TYR:OH	2.22	0.41
1:A:400:MET:CE	1:A:402:PRO:HG3	2.50	0.41
1:A:444:ARG:NH1	1:A:450:ARG:CD	2.83	0.41
1:B:79:LEU:HD21	1:B:362:ILE:CD1	2.43	0.41
1:A:50:GLN:O	1:A:52:ARG:N	2.54	0.40
1:B:36:HIS:O	1:B:38:TRP:N	2.53	0.40
1:A:330:GLU:HG2	1:A:383:ASP:H	1.85	0.40
1:A:376:TYR:OH	1:A:400:MET:HB2	2.20	0.40
1:B:220:LEU:HD23	1:B:220:LEU:HA	1.96	0.40
1:A:333:ARG:NE	1:A:370:GLN:O	2.41	0.40
1:A:68:TYR:O	1:A:363:ILE:N	2.47	0.40
1:A:86:HIS:HA	1:A:87:ILE:HD12	2.03	0.40
1:B:139:ALA:O	1:B:140:HIS:C	2.63	0.40
1:B:239:GLN:C	1:B:241:PRO:CD	2.94	0.40
1:B:244:LEU:CD1	1:B:271:ILE:HG21	2.52	0.40
1:A:68:TYR:OH	1:A:357:PRO:HG2	2.21	0.40
1:A:158:SER:OG	1:A:283:ILE:HG22	2.21	0.40
1:A:351:LEU:O	1:A:352:GLY:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:ASP:OD2	1:B:413:ASP:N	2.55	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	411/467 (88%)	317 (77%)	58 (14%)	36 (9%)	0	4
1	B	411/467 (88%)	326 (79%)	49 (12%)	36 (9%)	0	4
All	All	822/934 (88%)	643 (78%)	107 (13%)	72 (9%)	0	4

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	PRO
1	A	101	LYS
1	A	105	ALA
1	A	108	ASN
1	A	114	ARG
1	A	177	ASP
1	A	211	PRO
1	A	239	GLN
1	B	32	PRO
1	B	90	PRO
1	B	101	LYS
1	B	105	ALA
1	B	108	ASN
1	B	109	GLY
1	B	110	PRO
1	B	112	HIS
1	B	114	ARG

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Mol	Chain	Res	Type
1	B	177	ASP
1	B	211	PRO
1	B	239	GLN
1	A	35	GLY
1	A	89	GLY
1	A	107	ALA
1	A	109	GLY
1	A	110	PRO
1	A	115	GLN
1	A	163	VAL
1	A	379	ASN
1	B	35	GLY
1	B	51	LEU
1	B	107	ALA
1	B	315	PHE
1	B	379	ASN
1	A	51	LEU
1	A	112	HIS
1	A	113	ARG
1	A	186	ALA
1	A	243	ASP
1	A	396	PRO
1	B	115	GLN
1	B	236	ALA
1	B	241	PRO
1	B	310	GLY
1	B	396	PRO
1	A	90	PRO
1	A	162	ALA
1	A	213	ASN
1	A	241	PRO
1	A	310	GLY
1	A	315	PHE
1	A	321	LEU
1	B	44	PRO
1	B	213	ASN
1	B	218	ASP
1	B	275	GLY
1	B	321	LEU
1	A	124	ARG
1	A	236	ALA
1	A	319	ARG

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Mol	Chain	Res	Type
1	B	139	ALA
1	B	140	HIS
1	B	309	GLY
1	A	37	GLY
1	A	104	VAL
1	A	185	VAL
1	B	89	GLY
1	B	104	VAL
1	B	311	ARG
1	B	389	PRO
1	A	389	PRO
1	B	132	GLY
1	B	318	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	323/378 (85%)	279 (86%)	44 (14%)	3	16
1	B	323/378 (85%)	275 (85%)	48 (15%)	3	13
All	All	646/756 (85%)	554 (86%)	92 (14%)	3	14

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	32	PRO
1	A	33	LEU
1	A	34	LEU
1	A	52	ARG
1	A	66	THR
1	A	67	VAL
1	A	79	LEU
1	A	87	ILE
1	A	111	LEU

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Mol	Chain	Res	Type
1	A	126	ASP
1	A	157	GLU
1	A	158	SER
1	A	176	MET
1	A	178	GLU
1	A	187	LEU
1	A	211	PRO
1	A	223	LEU
1	A	225	LEU
1	A	226	LEU
1	A	231	ILE
1	A	235	ARG
1	A	239	GLN
1	A	241	PRO
1	A	243	ASP
1	A	248	LEU
1	A	264	ILE
1	A	267	GLN
1	A	268	VAL
1	A	279	ILE
1	A	301	ARG
1	A	305	GLU
1	A	308	THR
1	A	340	VAL
1	A	342	THR
1	A	350	GLU
1	A	351	LEU
1	A	362	ILE
1	A	389	PRO
1	A	402	PRO
1	A	403	PHE
1	A	408	ARG
1	A	445	VAL
1	A	459	VAL
1	B	31	VAL
1	B	32	PRO
1	B	33	LEU
1	B	34	LEU
1	B	51	LEU
1	B	66	THR
1	B	67	VAL
1	B	79	LEU

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Mol	Chain	Res	Type
1	B	87	ILE
1	B	111	LEU
1	B	117	ARG
1	B	126	ASP
1	B	151	THR
1	B	157	GLU
1	B	158	SER
1	B	174	GLN
1	B	176	MET
1	B	187	LEU
1	B	211	PRO
1	B	223	LEU
1	B	225	LEU
1	B	226	LEU
1	B	228	ASP
1	B	231	ILE
1	B	235	ARG
1	B	239	GLN
1	B	241	PRO
1	B	243	ASP
1	B	264	ILE
1	B	268	VAL
1	B	279	ILE
1	B	288	GLN
1	B	295	GLU
1	B	305	GLU
1	B	308	THR
1	B	340	VAL
1	B	342	THR
1	B	350	GLU
1	B	351	LEU
1	B	362	ILE
1	B	371	ARG
1	B	377	ASP
1	B	381	GLU
1	B	389	PRO
1	B	396	PRO
1	B	408	ARG
1	B	447	ILE
1	B	459	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	72	ASN
1	A	86	HIS
1	A	112	HIS
1	A	265	HIS
1	A	288	GLN
1	A	296	HIS
1	A	323	HIS
1	A	379	ASN
1	A	394	ASN
1	A	419	GLN
1	A	435	GLN
1	B	36	HIS
1	B	112	HIS
1	B	265	HIS
1	B	288	GLN
1	B	296	HIS
1	B	323	HIS
1	B	370	GLN
1	B	379	ASN
1	B	394	ASN
1	B	419	GLN
1	B	435	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	500	1	50,50,50	1.67	9 (18%)	67,82,82	1.03	4 (5%)
2	HEM	A	500	1	50,50,50	1.71	10 (20%)	67,82,82	1.10	6 (8%)
3	EL3	B	502	-	16,17,17	0.90	0	13,29,29	1.24	0
3	EL3	A	502	-	16,17,17	0.77	0	13,29,29	1.17	0
3	EL3	B	501	-	16,17,17	0.75	0	13,29,29	1.26	1 (7%)
3	EL3	A	501	-	16,17,17	0.80	0	13,29,29	1.14	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	B	500	1	-	6/14/54/54	-
2	HEM	A	500	1	-	7/14/54/54	-
3	EL3	B	502	-	-	-	0/4/3/3
3	EL3	A	502	-	-	-	0/4/3/3
3	EL3	B	501	-	-	-	0/4/3/3
3	EL3	A	501	-	-	-	0/4/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	CBC-CAC	4.92	1.54	1.30
2	A	500	HEM	CBC-CAC	4.92	1.54	1.30
2	B	500	HEM	CBB-CAB	4.74	1.53	1.30
2	A	500	HEM	CBB-CAB	4.63	1.52	1.30
2	B	500	HEM	CMC-C2C	3.20	1.57	1.50
2	A	500	HEM	CAC-C3C	3.03	1.55	1.47
2	B	500	HEM	CAB-C3B	2.98	1.55	1.47
2	B	500	HEM	CAC-C3C	2.91	1.55	1.47
2	A	500	HEM	CAB-C3B	2.85	1.55	1.47
2	A	500	HEM	FE-NA	2.79	2.04	1.95
2	A	500	HEM	CMC-C2C	2.63	1.56	1.50
2	A	500	HEM	CAA-C2A	2.54	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	FE-NA	2.52	2.03	1.95
2	A	500	HEM	CBA-CGA	2.35	1.56	1.50
2	B	500	HEM	FE-NB	2.35	2.02	1.94
2	A	500	HEM	CHA-C1A	-2.22	1.34	1.39
2	A	500	HEM	FE-NC	2.21	2.02	1.95
2	B	500	HEM	C1C-C2C	2.06	1.49	1.45
2	B	500	HEM	FE-NC	2.06	2.01	1.95

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	HEM	CAA-C2A-C3A	3.17	134.17	127.07
2	A	500	HEM	CBA-CAA-C2A	2.92	120.60	112.53
2	A	500	HEM	CBB-CAB-C3B	-2.85	113.30	127.53
2	B	500	HEM	CBB-CAB-C3B	-2.75	113.78	127.53
2	B	500	HEM	O1A-CGA-CBA	-2.69	114.55	123.09
2	A	500	HEM	O1A-CGA-CBA	-2.51	115.14	123.09
2	A	500	HEM	CAA-C2A-C1A	-2.49	120.08	124.94
2	B	500	HEM	CBC-CAC-C3C	-2.43	115.39	127.53
2	B	500	HEM	CAA-C2A-C3A	2.21	132.03	127.07
2	A	500	HEM	CBC-CAC-C3C	-2.16	116.72	127.53
3	B	501	EL3	CAG-CAH-CAO	-2.03	100.76	104.48

There are no chirality outliers.

All (13) torsion outliers are listed below:

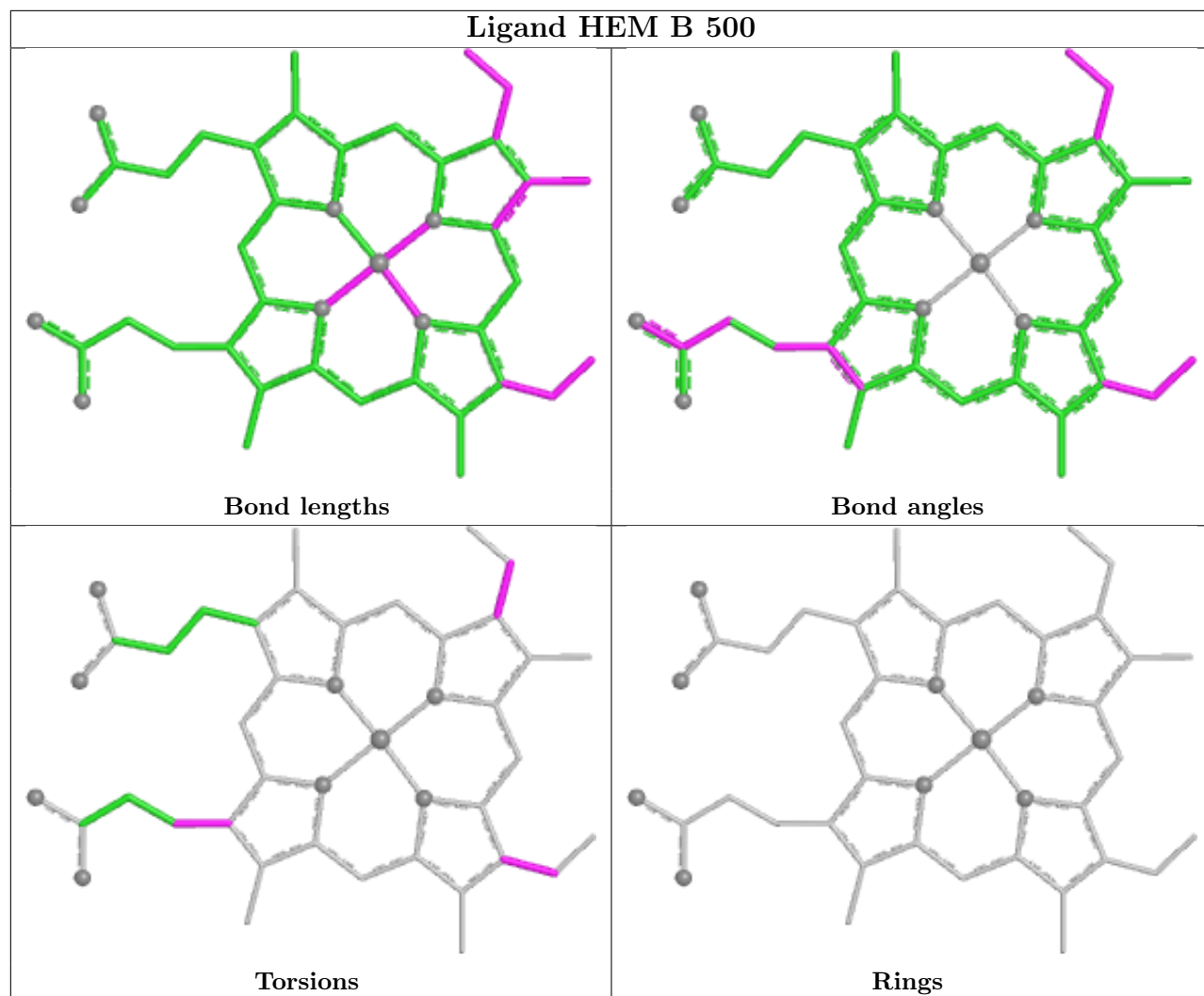
Mol	Chain	Res	Type	Atoms
2	A	500	HEM	C3A-C2A-CAA-CBA
2	A	500	HEM	C2B-C3B-CAB-CBB
2	A	500	HEM	C4B-C3B-CAB-CBB
2	B	500	HEM	C3A-C2A-CAA-CBA
2	B	500	HEM	C2B-C3B-CAB-CBB
2	B	500	HEM	C4B-C3B-CAB-CBB
2	B	500	HEM	C1A-C2A-CAA-CBA
2	A	500	HEM	C1A-C2A-CAA-CBA
2	B	500	HEM	C2C-C3C-CAC-CBC
2	B	500	HEM	C4C-C3C-CAC-CBC
2	A	500	HEM	CAA-CBA-CGA-O1A
2	A	500	HEM	CAA-CBA-CGA-O2A
2	A	500	HEM	C2C-C3C-CAC-CBC

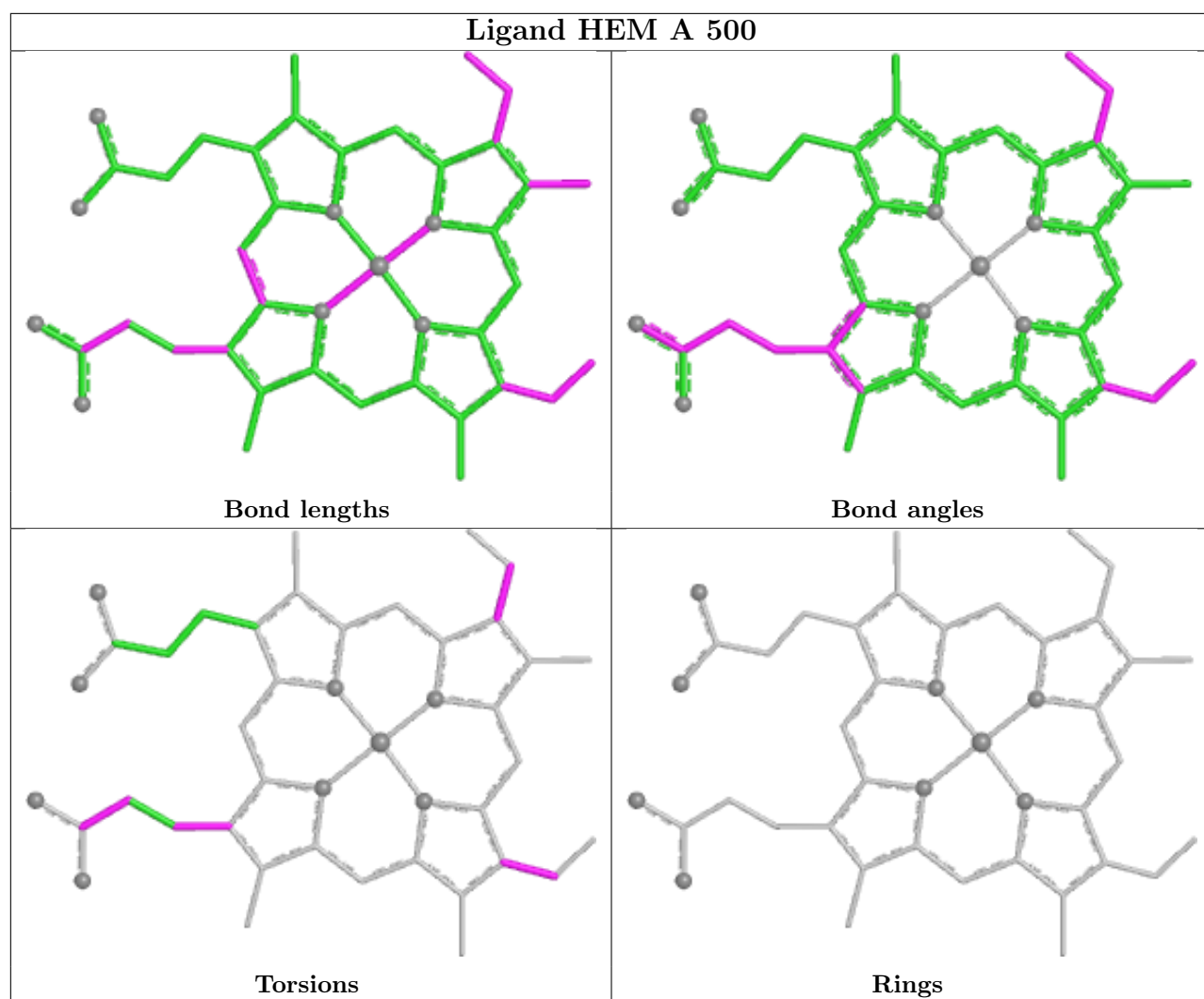
There are no ring outliers.

6 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	HEM	8	0
2	A	500	HEM	5	0
3	B	502	EL3	3	0
3	A	502	EL3	3	0
3	B	501	EL3	15	0
3	A	501	EL3	7	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 [i](#)

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

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	417/467 (89%)	-0.42	1 (0%) 91 86	14, 82, 127, 141	0
1	B	417/467 (89%)	-0.46	0 100 100	23, 83, 123, 141	0
All	All	834/934 (89%)	-0.44	1 (0%) 92 90	14, 83, 124, 141	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	VAL	2.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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.

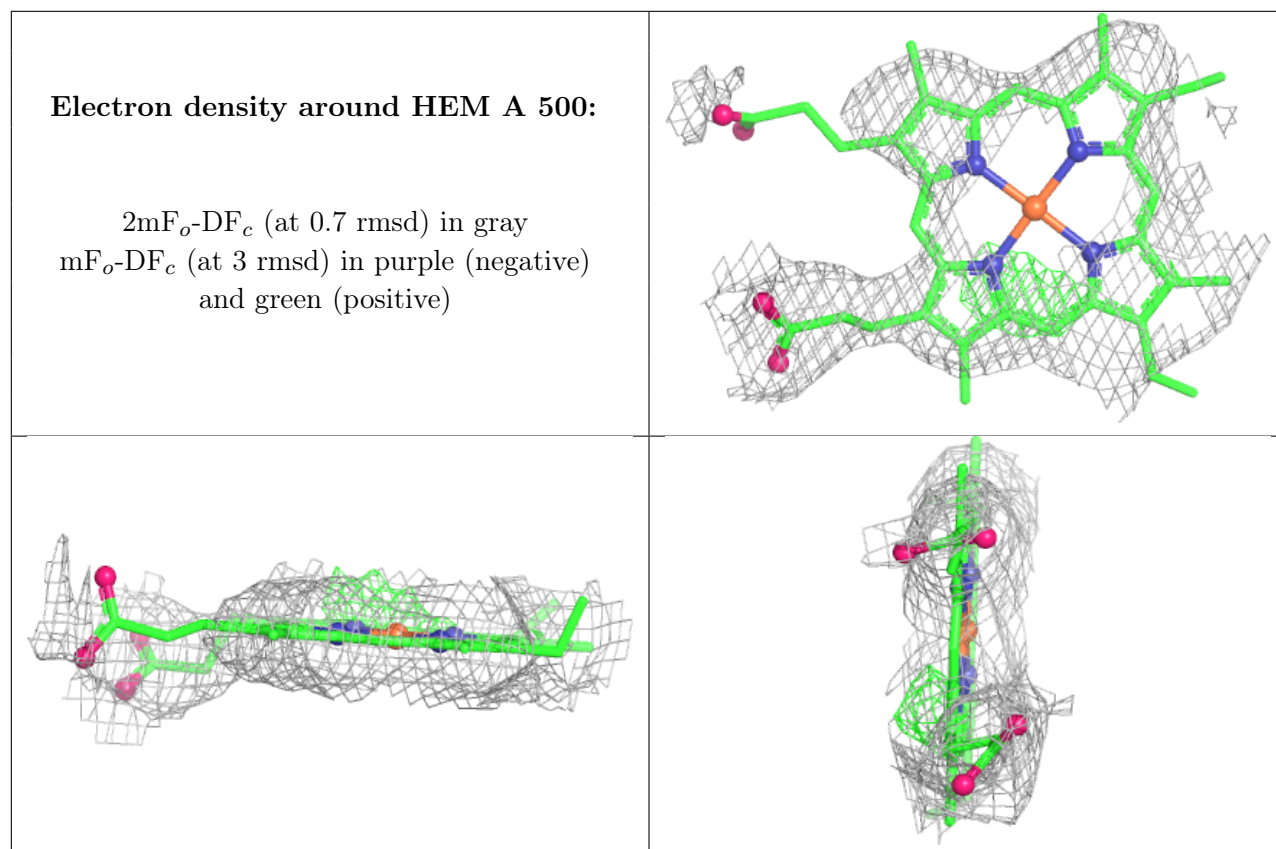
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EL3	A	502	15/15	0.96	0.10	112,114,114,115	0
3	EL3	B	502	15/15	0.96	0.11	100,101,102,102	0
3	EL3	B	501	15/15	0.97	0.13	99,100,100,101	0
3	EL3	A	501	15/15	0.97	0.14	91,91,92,92	0

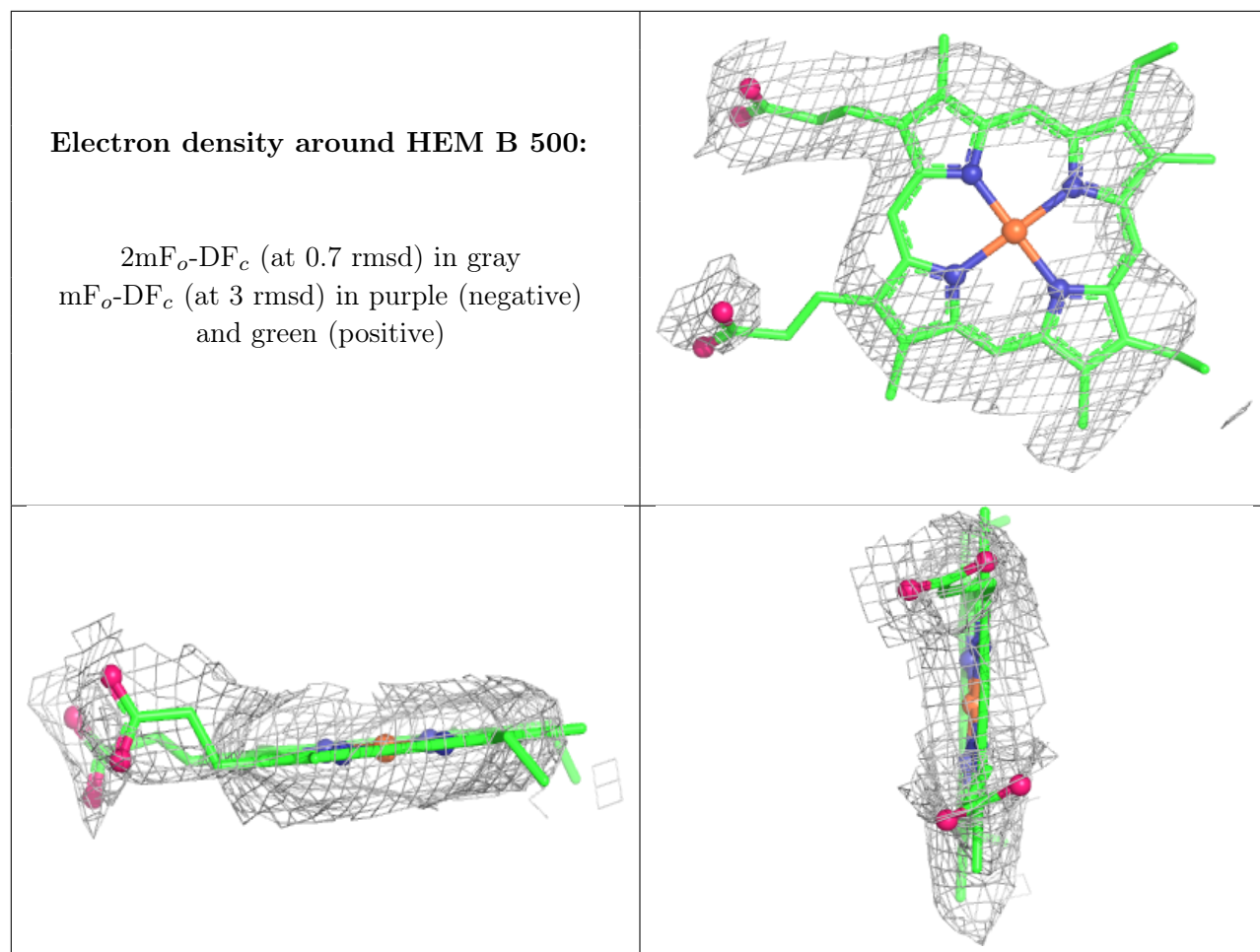
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	A	500	43/43	0.98	0.09	59,66,78,83	0
2	HEM	B	500	43/43	0.98	0.07	54,59,67,70	0

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.