



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:48 AM UTC

PDB ID : 4RUI / pdb_00004rui
Title : Crystal structure of a cytochrome P450 2A6 in complex with a monoterpene - sabinene.
Authors : Shah, M.B.; Stout, C.D.; Halpert, J.R.
Deposited on : 2014-11-19
Resolution : 2.61 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

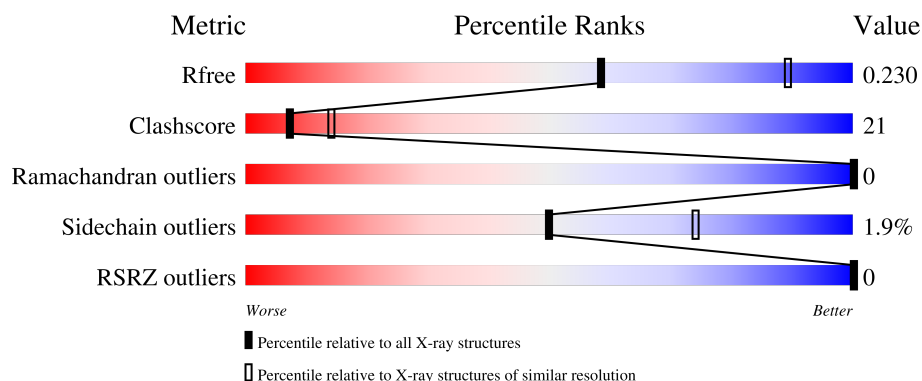
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	476	
1	B	476	
1	C	476	
1	D	476	
1	E	476	

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Mol	Chain	Length	Quality of chain
1	F	476	 71% 26%

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	SNE	C	502	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22515 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 2A6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	465	Total	C	N	O	S	0	0	0
			3688	2368	628	674	18			
1	A	464	Total	C	N	O	S	0	0	0
			3687	2369	627	673	18			
1	B	465	Total	C	N	O	S	0	0	0
			3692	2374	631	669	18			
1	C	464	Total	C	N	O	S	0	0	0
			3594	2313	598	665	18			
1	E	465	Total	C	N	O	S	0	0	0
			3627	2327	613	669	18			
1	F	465	Total	C	N	O	S	0	0	0
			3597	2320	593	666	18			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	23	MET	-	expression tag	UNP P11509
D	24	ALA	-	expression tag	UNP P11509
D	25	LYS	-	expression tag	UNP P11509
D	26	LYS	-	expression tag	UNP P11509
D	27	THR	-	expression tag	UNP P11509
D	28	SER	-	expression tag	UNP P11509
D	392	TYR	PHE	variant	UNP P11509
D	495	HIS	-	expression tag	UNP P11509
D	496	HIS	-	expression tag	UNP P11509
D	497	HIS	-	expression tag	UNP P11509
D	498	HIS	-	expression tag	UNP P11509
A	23	MET	-	expression tag	UNP P11509
A	24	ALA	-	expression tag	UNP P11509
A	25	LYS	-	expression tag	UNP P11509
A	26	LYS	-	expression tag	UNP P11509
A	27	THR	-	expression tag	UNP P11509
A	28	SER	-	expression tag	UNP P11509

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Chain	Residue	Modelled	Actual	Comment	Reference
A	392	TYR	PHE	variant	UNP P11509
A	495	HIS	-	expression tag	UNP P11509
A	496	HIS	-	expression tag	UNP P11509
A	497	HIS	-	expression tag	UNP P11509
A	498	HIS	-	expression tag	UNP P11509
B	23	MET	-	expression tag	UNP P11509
B	24	ALA	-	expression tag	UNP P11509
B	25	LYS	-	expression tag	UNP P11509
B	26	LYS	-	expression tag	UNP P11509
B	27	THR	-	expression tag	UNP P11509
B	28	SER	-	expression tag	UNP P11509
B	392	TYR	PHE	variant	UNP P11509
B	495	HIS	-	expression tag	UNP P11509
B	496	HIS	-	expression tag	UNP P11509
B	497	HIS	-	expression tag	UNP P11509
B	498	HIS	-	expression tag	UNP P11509
C	23	MET	-	expression tag	UNP P11509
C	24	ALA	-	expression tag	UNP P11509
C	25	LYS	-	expression tag	UNP P11509
C	26	LYS	-	expression tag	UNP P11509
C	27	THR	-	expression tag	UNP P11509
C	28	SER	-	expression tag	UNP P11509
C	392	TYR	PHE	variant	UNP P11509
C	495	HIS	-	expression tag	UNP P11509
C	496	HIS	-	expression tag	UNP P11509
C	497	HIS	-	expression tag	UNP P11509
C	498	HIS	-	expression tag	UNP P11509
E	23	MET	-	expression tag	UNP P11509
E	24	ALA	-	expression tag	UNP P11509
E	25	LYS	-	expression tag	UNP P11509
E	26	LYS	-	expression tag	UNP P11509
E	27	THR	-	expression tag	UNP P11509
E	28	SER	-	expression tag	UNP P11509
E	392	TYR	PHE	variant	UNP P11509
E	495	HIS	-	expression tag	UNP P11509
E	496	HIS	-	expression tag	UNP P11509
E	497	HIS	-	expression tag	UNP P11509
E	498	HIS	-	expression tag	UNP P11509
F	23	MET	-	expression tag	UNP P11509
F	24	ALA	-	expression tag	UNP P11509
F	25	LYS	-	expression tag	UNP P11509
F	26	LYS	-	expression tag	UNP P11509

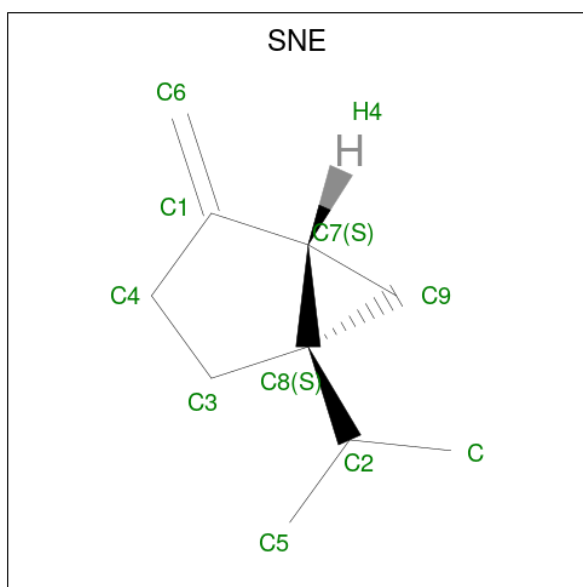
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Chain	Residue	Modelled	Actual	Comment	Reference
F	27	THR	-	expression tag	UNP P11509
F	28	SER	-	expression tag	UNP P11509
F	392	TYR	PHE	variant	UNP P11509
F	495	HIS	-	expression tag	UNP P11509
F	496	HIS	-	expression tag	UNP P11509
F	497	HIS	-	expression tag	UNP P11509
F	498	HIS	-	expression tag	UNP P11509

- # HEM

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C 10 10	0	0
3	A	1	Total C 10 10	0	0
3	B	1	Total C 10 10	0	0
3	C	1	Total C 10 10	0	0
3	E	1	Total C 10 10	0	0
3	F	1	Total C 10 10	0	0

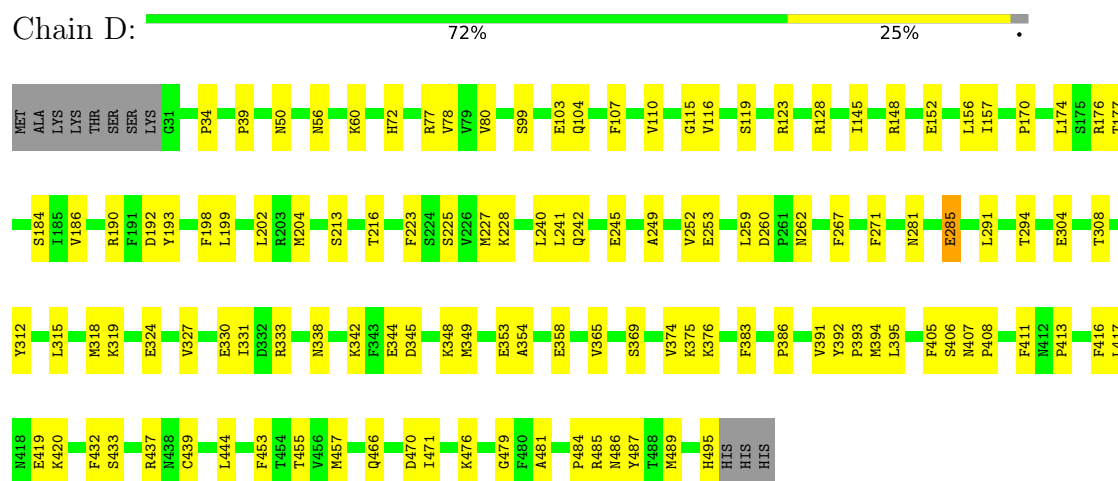
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	53	Total O 53 53	0	0
4	A	74	Total O 74 74	0	0
4	B	65	Total O 65 65	0	0
4	C	36	Total O 36 36	0	0
4	E	46	Total O 46 46	0	0
4	F	38	Total O 38 38	0	0

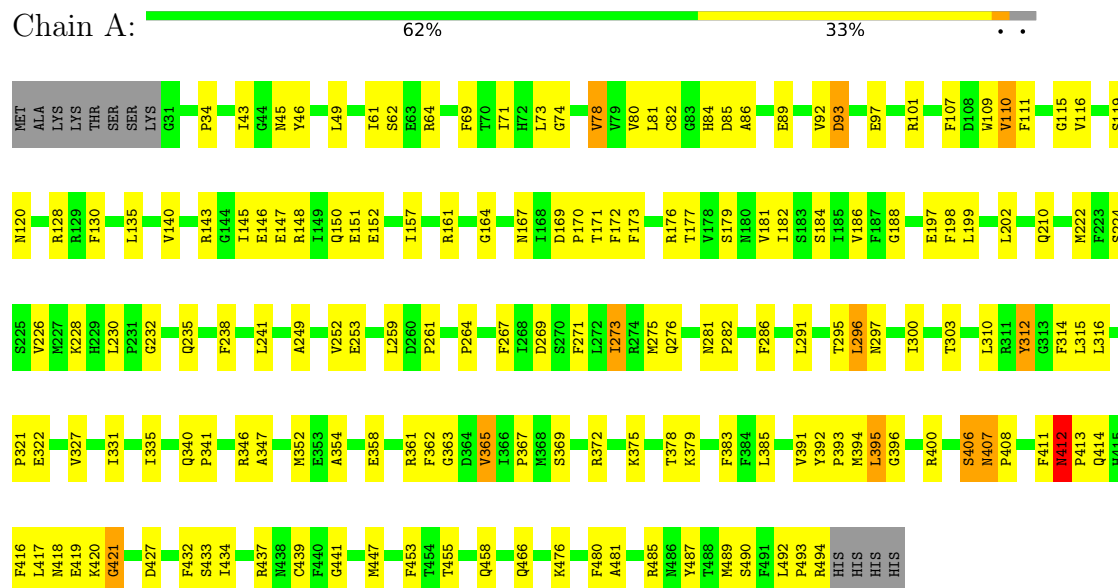
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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 2A6

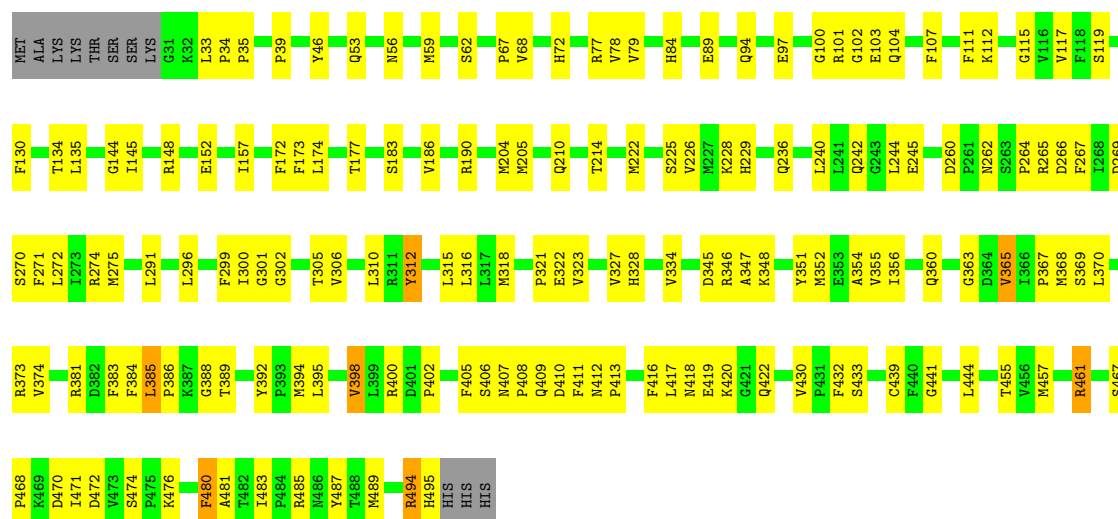


• Molecule 1: Cytochrome P450 2A6



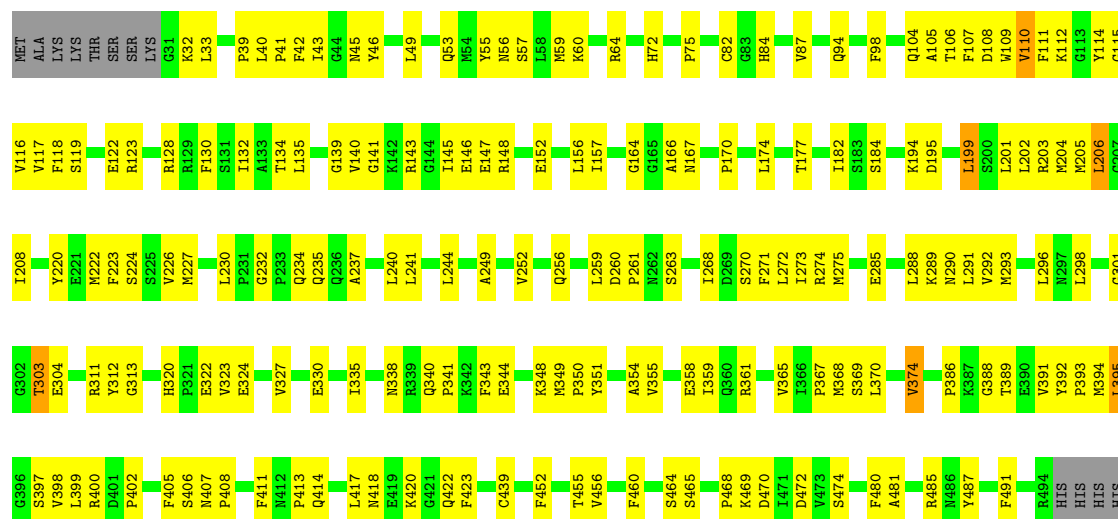
• Molecule 1: Cytochrome P450 2A6

Chain B:  64% 32% ..



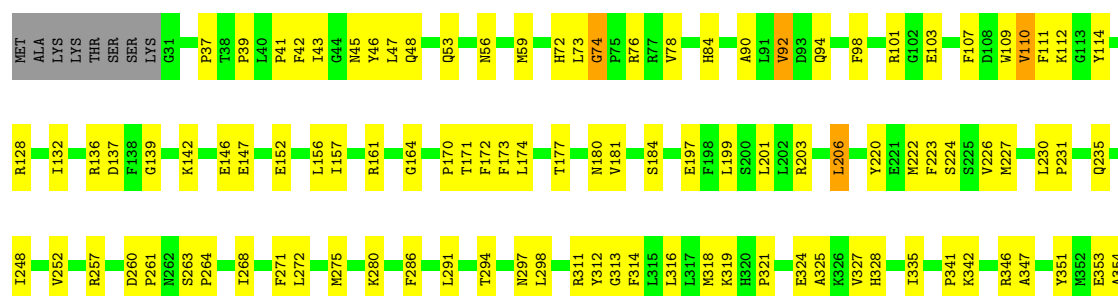
• Molecule 1: Cytochrome P450 2A6

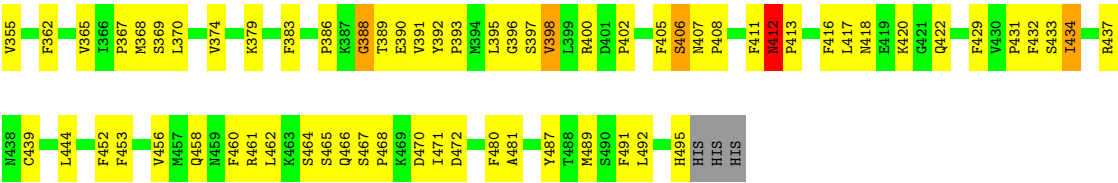
Chain C:  58% 38% ..



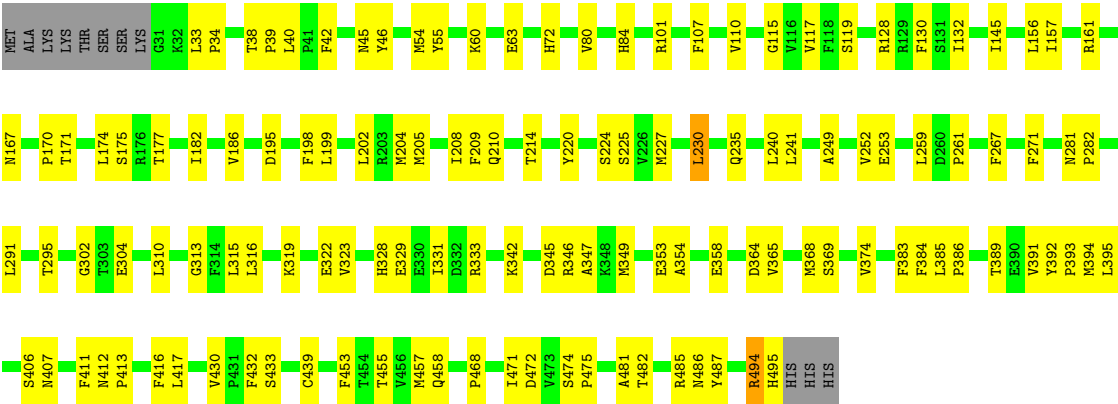
• Molecule 1: Cytochrome P450 2A6

Chain E:  62% 33% ..





• Molecule 1: Cytochrome P450 2A6



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.74Å 132.97Å 133.03Å 62.40° 99.06° 80.93°	Depositor
Resolution (Å)	50.00 – 2.61 50.00 – 2.61	Depositor EDS
% Data completeness (in resolution range)	90.2 (50.00-2.61) 90.0 (50.00-2.61)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.197 , 0.261 0.206 , 0.230	Depositor DCC
R_{free} test set	5003 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.417 for h,-l,-h+k-l 0.417 for h,h-k+l,-k 0.032 for -h,-h+k-l,-l 0.029 for -h,l,k 0.030 for -h,-k,h-k+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22515	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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, SNE

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	0.87	2/3778 (0.1%)	1.07	12/5105 (0.2%)
1	B	0.82	0/3784	1.07	16/5113 (0.3%)
1	C	0.82	1/3684 (0.0%)	1.08	9/4997 (0.2%)
1	D	0.79	0/3780	1.01	5/5112 (0.1%)
1	E	0.82	2/3717 (0.1%)	1.00	9/5034 (0.2%)
1	F	0.78	0/3689	1.01	9/5005 (0.2%)
All	All	0.82	5/22432 (0.0%)	1.04	60/30366 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	110	VAL	CA-CB	-6.19	1.48	1.55
1	A	43	ILE	CA-CB	-5.82	1.48	1.54
1	E	110	VAL	CA-CB	-5.37	1.47	1.55
1	E	406	SER	C-O	-5.25	1.17	1.24
1	A	406	SER	CA-C	-5.18	1.46	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	43	ILE	N-CA-C	-12.83	100.51	113.47
1	C	395	LEU	N-CA-C	-9.57	101.16	113.12
1	A	226	VAL	N-CA-C	-9.38	104.24	112.12
1	B	226	VAL	N-CA-C	-9.21	104.44	111.90
1	E	110	VAL	CB-CA-C	-8.14	103.81	111.05
1	C	338	ASN	N-CA-C	7.72	119.60	111.03
1	F	412	ASN	CA-C-N	7.58	127.25	119.82
1	F	412	ASN	C-N-CA	7.58	127.25	119.82
1	B	385	LEU	CA-C-N	7.49	127.49	119.78
1	B	385	LEU	C-N-CA	7.49	127.49	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	344	GLU	N-CA-C	-7.39	104.24	113.18
1	A	365	VAL	N-CA-C	6.63	116.78	110.42
1	D	348	LYS	CA-C-N	-6.30	115.53	123.15
1	D	348	LYS	C-N-CA	-6.30	115.53	123.15
1	F	407	ASN	CA-C-N	6.30	126.50	119.32
1	F	407	ASN	C-N-CA	6.30	126.50	119.32
1	F	406	SER	CA-C-N	-6.30	115.41	123.16
1	F	406	SER	C-N-CA	-6.30	115.41	123.16
1	E	43	ILE	N-CA-C	-6.25	107.03	113.10
1	B	494	ARG	N-CA-C	6.11	119.20	109.24
1	A	407	ASN	CA-C-N	6.08	125.97	119.28
1	A	407	ASN	C-N-CA	6.08	125.97	119.28
1	C	110	VAL	O-C-N	-6.01	116.63	121.98
1	B	406	SER	CA-C-N	-5.88	116.03	123.15
1	B	406	SER	C-N-CA	-5.88	116.03	123.15
1	C	232	GLY	CA-C-N	5.68	124.88	118.97
1	C	232	GLY	C-N-CA	5.68	124.88	118.97
1	B	67	PRO	CA-C-N	-5.65	117.59	122.96
1	B	67	PRO	C-N-CA	-5.65	117.59	122.96
1	D	78	VAL	N-CA-C	5.58	115.93	108.11
1	F	494	ARG	N-CA-C	5.58	117.03	109.11
1	A	421	GLY	N-CA-C	5.46	121.45	113.48
1	A	314	PHE	N-CA-C	-5.44	105.43	111.36
1	F	385	LEU	CA-C-N	5.42	126.62	119.84
1	F	385	LEU	C-N-CA	5.42	126.62	119.84
1	B	412	ASN	CA-C-N	5.42	125.13	119.82
1	B	412	ASN	C-N-CA	5.42	125.13	119.82
1	E	388	GLY	N-CA-C	5.41	122.78	115.32
1	B	480	PHE	N-CA-C	-5.40	105.82	112.90
1	B	461	ARG	N-CA-C	-5.39	101.38	109.95
1	A	412	ASN	CA-C-N	5.38	126.57	119.84
1	A	412	ASN	C-N-CA	5.38	126.57	119.84
1	E	74	GLY	N-CA-C	-5.38	101.38	112.34
1	D	338	ASN	N-CA-C	5.35	122.19	110.80
1	C	256	GLN	N-CA-C	-5.31	105.14	111.03
1	B	398	VAL	N-CA-C	-5.28	105.25	111.00
1	C	110	VAL	CB-CA-C	-5.28	106.43	111.44
1	A	93	ASP	N-CA-C	-5.27	106.69	113.23
1	A	447	MET	N-CA-C	-5.22	105.50	111.14
1	A	395	LEU	N-CA-C	-5.21	105.67	112.23
1	E	412	ASN	CA-C-N	5.20	124.86	119.56
1	E	412	ASN	C-N-CA	5.20	124.86	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	398	VAL	CB-CA-C	-5.17	105.27	112.04
1	E	465	SER	N-CA-C	-5.14	106.98	113.20
1	E	92	VAL	N-CA-C	5.13	116.06	111.90
1	B	430	VAL	CA-C-N	-5.11	114.40	119.56
1	B	430	VAL	C-N-CA	-5.11	114.40	119.56
1	A	78	VAL	N-CA-C	5.10	115.46	108.12
1	C	312	TYR	N-CA-C	-5.04	105.87	111.36
1	B	365	VAL	N-CA-C	5.01	115.23	110.42

There are no chirality outliers.

There are no planarity outliers.

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	3687	0	3585	163	0
1	B	3692	0	3591	125	0
1	C	3594	0	3388	193	0
1	D	3688	0	3560	106	0
1	E	3627	0	3441	178	0
1	F	3597	0	3372	117	0
2	A	43	0	30	12	0
2	B	43	0	30	17	0
2	C	43	0	30	3	0
2	D	43	0	30	15	0
2	E	43	0	30	10	0
2	F	43	0	30	13	0
3	A	10	0	16	1	0
3	B	10	0	16	2	0
3	C	10	0	16	6	0
3	D	10	0	16	1	0
3	E	10	0	16	4	0
3	F	10	0	16	3	0
4	A	74	0	0	12	0
4	B	65	0	0	8	0
4	C	36	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	53	0	0	7	0
4	E	46	0	0	5	0
4	F	38	0	0	1	0
All	All	22515	0	21213	894	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 21.

All (894) 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:F:354:ALA:CB	1:F:417:LEU:HD21	1.62	1.30
1:C:40:LEU:HB3	1:C:41:PRO:CD	1.66	1.26
1:E:107:PHE:O	1:E:110:VAL:HG12	1.30	1.25
1:A:439:CYS:HB2	2:A:502:HEM:NA	1.57	1.17
1:E:354:ALA:CB	1:E:417:LEU:HD21	1.77	1.15
1:C:330:GLU:OE2	1:C:351:TYR:HB3	1.43	1.14
1:C:139:GLY:HA3	1:C:145:ILE:HG23	1.24	1.14
1:C:140:VAL:HA	1:C:145:ILE:HD13	1.21	1.11
1:D:354:ALA:CB	1:D:417:LEU:CD1	2.29	1.11
1:A:49:LEU:HD21	1:A:71:ILE:HD11	1.18	1.10
1:F:354:ALA:CB	1:F:417:LEU:CD2	2.31	1.08
1:D:354:ALA:CB	1:D:417:LEU:HD11	1.83	1.08
1:A:111:PHE:CZ	1:A:296:LEU:HD12	1.88	1.08
1:A:115:GLY:O	1:A:119:SER:HB3	1.53	1.06
1:A:439:CYS:HB2	2:A:502:HEM:C1A	1.90	1.06
1:C:40:LEU:HB3	1:C:41:PRO:HD2	1.09	1.05
1:F:354:ALA:HB1	1:F:417:LEU:CD2	1.85	1.05
1:A:327:VAL:HG13	1:A:352:MET:HE1	1.37	1.05
1:B:419:GLU:HA	4:B:613:HOH:O	1.54	1.05
1:E:230:LEU:HD22	1:E:231:PRO:HD2	1.37	1.05
1:F:209:PHE:CE2	1:F:304:GLU:HB3	1.92	1.05
1:E:223:PHE:O	1:E:227:MET:HG3	1.59	1.03
2:D:501:HEM:HBC2	2:D:501:HEM:HMC2	1.39	1.02
1:D:39:PRO:HG3	1:D:72:HIS:CE1	1.94	1.02
1:D:312:TYR:CD2	1:D:484:PRO:HB3	1.95	1.01
1:B:439:CYS:HB2	2:B:501:HEM:NA	1.75	0.99
1:A:49:LEU:HD21	1:A:71:ILE:CD1	1.93	0.99
1:C:249:ALA:O	1:C:252:VAL:HG12	1.62	0.99
1:C:206:LEU:HD13	1:C:206:LEU:O	1.62	0.99
1:D:123:ARG:HA	1:D:285:GLU:HG3	1.41	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:LEU:HD13	1:E:206:LEU:O	1.64	0.96
1:C:439:CYS:HB2	2:C:501:HEM:NA	1.79	0.96
1:A:157:ILE:HD11	1:A:455:THR:HG22	1.47	0.96
1:E:110:VAL:HG13	1:E:111:PHE:CD1	2.01	0.96
1:C:139:GLY:CA	1:C:145:ILE:HG23	1.95	0.96
1:A:249:ALA:O	1:A:252:VAL:HG12	1.64	0.95
1:A:354:ALA:CB	1:A:417:LEU:HD21	1.96	0.95
1:B:327:VAL:HG13	1:B:352:MET:CE	1.98	0.94
1:E:110:VAL:CG1	1:E:111:PHE:CD1	2.51	0.94
1:A:86:ALA:HB3	4:A:658:HOH:O	1.67	0.94
1:B:115:GLY:O	1:B:119:SER:HB3	1.69	0.93
1:A:378:THR:CG2	1:A:385:LEU:HB2	1.98	0.93
1:E:354:ALA:CB	1:E:417:LEU:CD2	2.47	0.93
1:A:413:PRO:O	1:A:417:LEU:HD23	1.70	0.92
2:A:502:HEM:HMC2	2:A:502:HEM:HBC2	1.48	0.92
1:D:354:ALA:HB1	1:D:417:LEU:CD1	1.98	0.91
1:D:192:ASP:HA	4:D:633:HOH:O	1.70	0.91
1:E:110:VAL:HG13	1:E:111:PHE:N	1.82	0.91
1:B:327:VAL:CG1	1:B:352:MET:HE1	2.00	0.91
1:E:37:PRO:HB2	1:E:48:GLN:OE1	1.71	0.91
1:C:301:GLY:HA2	3:C:502:SNE:H12	1.53	0.90
1:E:354:ALA:HB1	1:E:417:LEU:CD2	2.01	0.90
1:F:354:ALA:HB1	1:F:417:LEU:HD21	1.43	0.90
1:C:237:ALA:O	1:C:241:LEU:HD23	1.71	0.89
1:A:327:VAL:HG13	1:A:352:MET:CE	2.02	0.89
1:D:342:LYS:O	1:D:345:ASP:HB2	1.72	0.89
2:D:501:HEM:HMB1	2:D:501:HEM:HBB2	1.52	0.89
1:A:111:PHE:HZ	1:A:296:LEU:HD12	1.35	0.89
1:B:439:CYS:HB2	2:B:501:HEM:C1A	2.07	0.89
1:B:225:SER:HA	1:B:228:LYS:HE3	1.55	0.89
1:C:40:LEU:CB	1:C:41:PRO:CD	2.49	0.88
1:E:92:VAL:HG23	1:E:434:ILE:HD12	1.54	0.88
1:E:206:LEU:HD13	1:E:206:LEU:C	1.98	0.88
1:C:170:PRO:HB2	1:C:174:LEU:HD23	1.55	0.88
1:B:461:ARG:HD3	4:B:616:HOH:O	1.72	0.87
1:D:354:ALA:HB2	1:D:417:LEU:CD1	2.02	0.87
1:E:107:PHE:CE2	3:E:502:SNE:H7	2.09	0.87
1:E:439:CYS:HB2	2:E:501:HEM:NA	1.89	0.86
1:C:140:VAL:HA	1:C:145:ILE:CD1	2.04	0.86
1:D:345:ASP:O	1:D:349:MET:HG3	1.76	0.85
1:A:109:TRP:CE3	1:A:110:VAL:HG23	2.11	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:492:LEU:HD12	1:E:492:LEU:N	1.90	0.85
1:F:209:PHE:CD2	1:F:304:GLU:HG3	2.11	0.85
1:C:206:LEU:HD13	1:C:206:LEU:C	2.01	0.85
1:F:413:PRO:O	1:F:417:LEU:HD23	1.77	0.85
1:A:354:ALA:CB	1:A:417:LEU:CD2	2.54	0.85
1:E:354:ALA:HB1	1:E:417:LEU:HD21	1.57	0.84
1:C:354:ALA:CB	1:C:417:LEU:CD2	2.56	0.84
1:E:109:TRP:CE3	1:E:109:TRP:O	2.30	0.84
1:A:181:VAL:O	1:A:184:SER:HB2	1.76	0.84
1:B:413:PRO:O	1:B:417:LEU:HD23	1.78	0.84
1:F:495:HIS:O	1:F:495:HIS:CD2	2.30	0.84
1:A:111:PHE:CE2	1:A:296:LEU:HD12	2.12	0.83
1:C:370:LEU:HD21	3:C:502:SNE:H5	1.60	0.83
1:B:327:VAL:HG13	1:B:352:MET:HE2	1.58	0.83
1:F:249:ALA:O	1:F:252:VAL:HG12	1.77	0.83
1:D:312:TYR:CE2	1:D:484:PRO:HB3	2.14	0.83
1:C:140:VAL:CA	1:C:145:ILE:HD13	2.05	0.83
1:C:354:ALA:CB	1:C:417:LEU:HD21	2.08	0.83
1:A:354:ALA:HB1	1:A:417:LEU:CD2	2.10	0.82
1:C:117:VAL:HG12	1:C:118:PHE:CD1	2.15	0.81
1:F:110:VAL:HG11	1:F:241:LEU:HD22	1.62	0.81
2:D:501:HEM:HBC2	2:D:501:HEM:CMC	2.10	0.81
1:C:109:TRP:HE3	1:C:110:VAL:CG2	1.94	0.81
1:A:86:ALA:CB	4:A:658:HOH:O	2.26	0.80
1:E:354:ALA:HB2	1:E:417:LEU:HD21	1.62	0.80
1:F:392:TYR:HB3	1:F:394:MET:HE3	1.63	0.79
1:A:327:VAL:CG1	1:A:352:MET:HE1	2.13	0.79
1:D:110:VAL:HG11	1:D:241:LEU:HD22	1.65	0.79
1:E:107:PHE:O	1:E:110:VAL:CG1	2.23	0.79
1:C:199:LEU:C	1:C:199:LEU:HD13	2.07	0.78
1:F:354:ALA:HB2	1:F:417:LEU:HD21	1.62	0.78
2:D:501:HEM:HBB2	2:D:501:HEM:CMB	2.13	0.78
1:A:249:ALA:O	1:A:252:VAL:CG1	2.30	0.78
1:C:204:MET:HA	1:C:240:LEU:HD22	1.65	0.78
1:A:111:PHE:CZ	1:A:296:LEU:CD1	2.66	0.78
1:F:374:VAL:HG21	1:F:386:PRO:O	1.84	0.78
1:C:330:GLU:OE2	1:C:351:TYR:CB	2.27	0.77
1:B:444:LEU:HD23	2:B:501:HEM:HBC2	1.64	0.77
1:A:249:ALA:C	1:A:252:VAL:HG12	2.08	0.77
1:B:354:ALA:CB	1:B:417:LEU:HD21	2.15	0.77
1:D:354:ALA:HB1	1:D:417:LEU:HD13	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:474:SER:HB3	1:F:485:ARG:HH21	1.50	0.77
1:A:111:PHE:HZ	1:A:296:LEU:CD1	1.96	0.77
1:F:354:ALA:HB2	1:F:417:LEU:CD2	2.14	0.77
1:E:152:GLU:HG3	1:E:177:THR:HG23	1.66	0.77
1:E:391:VAL:O	1:E:393:PRO:HD3	1.84	0.77
1:E:170:PRO:HB2	1:E:174:LEU:HD23	1.67	0.76
1:A:109:TRP:HE3	1:A:110:VAL:HG23	1.48	0.76
1:A:249:ALA:HA	1:A:252:VAL:HG12	1.67	0.76
1:B:244:LEU:HB3	1:B:296:LEU:HD11	1.66	0.76
1:E:73:LEU:O	1:E:76:ARG:HG3	1.85	0.76
1:E:37:PRO:CB	1:E:48:GLN:OE1	2.34	0.76
1:F:175:SER:HB3	1:F:202:LEU:HD22	1.67	0.76
1:D:439:CYS:HB2	2:D:501:HEM:NA	1.99	0.76
1:F:358:GLU:HG3	1:F:411:PHE:CE1	2.20	0.76
1:C:32:LYS:HG3	1:C:33:LEU:H	1.50	0.76
1:E:374:VAL:HG21	1:E:386:PRO:O	1.85	0.76
1:F:271:PHE:CE2	1:F:291:LEU:HB2	2.20	0.76
1:C:139:GLY:O	1:C:145:ILE:HG12	1.86	0.75
1:E:491:PHE:C	1:E:492:LEU:HD12	2.10	0.75
1:C:139:GLY:HA3	1:C:145:ILE:CG2	2.12	0.75
1:D:374:VAL:HG22	1:D:376:LYS:O	1.86	0.75
1:D:444:LEU:HD23	2:D:501:HEM:CBC	2.17	0.75
1:F:494:ARG:O	1:F:495:HIS:C	2.30	0.75
1:D:416:PHE:O	1:D:417:LEU:HD12	1.86	0.74
1:B:327:VAL:CG1	1:B:352:MET:CE	2.63	0.74
1:C:40:LEU:CB	1:C:41:PRO:HD2	2.04	0.74
1:C:130:PHE:CE2	1:C:274:ARG:HD3	2.22	0.74
1:C:109:TRP:CE3	1:C:110:VAL:HG22	2.23	0.74
1:F:209:PHE:CD2	1:F:304:GLU:CG	2.70	0.74
1:E:405:PHE:HA	4:E:613:HOH:O	1.86	0.73
1:C:39:PRO:HG3	1:C:72:HIS:ND1	2.02	0.73
1:C:348:LYS:O	1:C:350:PRO:HD2	1.89	0.72
1:C:109:TRP:HE3	1:C:110:VAL:HG23	1.52	0.72
1:C:330:GLU:OE1	1:C:349:MET:CA	2.38	0.72
1:A:392:TYR:HB3	1:A:394:MET:CE	2.20	0.72
1:D:39:PRO:HB3	1:D:72:HIS:ND1	2.05	0.72
1:E:110:VAL:CG1	1:E:111:PHE:N	2.52	0.72
1:E:206:LEU:C	1:E:206:LEU:CD1	2.63	0.71
1:D:407:ASN:N	1:D:408:PRO:HD3	2.04	0.71
1:E:313:GLY:HA3	1:E:453:PHE:HZ	1.56	0.71
1:C:199:LEU:HD11	1:C:203:ARG:NE	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ARG:HG2	1:A:198:PHE:CE2	2.25	0.71
1:C:139:GLY:C	1:C:145:ILE:HG23	2.15	0.71
1:C:418:ASN:OD1	1:C:418:ASN:C	2.31	0.71
1:A:458:GLN:HA	1:A:494:ARG:HH12	1.54	0.71
1:C:40:LEU:HD12	1:C:41:PRO:HD3	1.73	0.70
1:F:182:ILE:HD13	2:F:501:HEM:HBC1	1.72	0.70
1:D:312:TYR:CD2	1:D:484:PRO:CB	2.74	0.70
1:C:392:TYR:HB3	1:C:394:MET:HE3	1.73	0.70
1:F:230:LEU:O	1:F:235:GLN:NE2	2.20	0.70
1:E:109:TRP:O	1:E:109:TRP:CD2	2.45	0.70
1:A:378:THR:HG23	1:A:385:LEU:HB2	1.70	0.69
1:B:444:LEU:HD23	2:B:501:HEM:CBC	2.22	0.69
2:F:501:HEM:CMB	2:F:501:HEM:HBB2	2.22	0.69
1:C:109:TRP:CE3	1:C:110:VAL:CG2	2.75	0.69
1:A:148:ARG:NH2	1:A:152:GLU:OE2	2.26	0.69
1:C:208:ILE:HG12	1:C:241:LEU:HD22	1.75	0.69
1:C:354:ALA:HB2	1:C:417:LEU:CD2	2.22	0.69
2:F:501:HEM:HBB2	2:F:501:HEM:HMB2	1.74	0.69
1:E:76:ARG:NH2	1:E:390:GLU:OE2	2.25	0.68
1:F:107:PHE:O	1:F:110:VAL:HG12	1.92	0.68
1:E:374:VAL:HG23	1:E:388:GLY:H	1.57	0.68
1:C:123:ARG:HA	1:C:285:GLU:HG3	1.74	0.68
1:E:128:ARG:O	1:E:132:ILE:HG13	1.93	0.68
1:E:432:PHE:CE1	2:E:501:HEM:HBB2	2.28	0.68
1:E:492:LEU:N	1:E:492:LEU:CD1	2.55	0.68
1:B:345:ASP:HA	1:B:348:LYS:HE2	1.76	0.68
1:A:249:ALA:CA	1:A:252:VAL:HG12	2.23	0.68
1:C:128:ARG:O	1:C:132:ILE:HG13	1.93	0.68
1:E:406:SER:O	1:E:407:ASN:HB2	1.93	0.68
1:D:170:PRO:HB2	1:D:174:LEU:HD23	1.75	0.67
1:F:209:PHE:HD2	1:F:304:GLU:HG3	1.59	0.67
1:B:354:ALA:HB1	1:B:417:LEU:CD2	2.24	0.67
1:C:330:GLU:OE1	1:C:349:MET:HA	1.94	0.67
1:D:34:PRO:HD3	1:D:383:PHE:HB3	1.76	0.67
1:B:368:MET:HB2	4:B:664:HOH:O	1.94	0.67
1:F:439:CYS:HB2	2:F:501:HEM:NA	2.10	0.66
1:A:458:GLN:HA	1:A:494:ARG:NH1	2.10	0.66
1:C:110:VAL:HG21	1:C:241:LEU:HB3	1.76	0.66
1:C:439:CYS:HB2	2:C:501:HEM:C1A	2.29	0.66
1:E:354:ALA:HB2	1:E:417:LEU:CD2	2.22	0.66
1:B:210:GLN:O	1:B:214:THR:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:VAL:CG1	1:C:118:PHE:CD1	2.78	0.66
1:C:224:SER:C	1:C:226:VAL:H	2.04	0.66
1:C:350:PRO:HB3	1:C:423:PHE:HB2	1.77	0.66
1:E:197:GLU:O	1:E:201:LEU:HD13	1.96	0.66
1:C:111:PHE:HA	1:C:293:MET:HE3	1.78	0.66
1:C:139:GLY:C	1:C:145:ILE:CG2	2.69	0.65
1:C:472:ASP:OD1	1:C:472:ASP:C	2.38	0.65
1:C:206:LEU:C	1:C:206:LEU:CD1	2.69	0.65
1:D:354:ALA:HB3	1:D:417:LEU:HD11	1.76	0.65
1:A:249:ALA:HA	1:A:252:VAL:CG1	2.26	0.65
1:C:195:ASP:C	1:C:195:ASP:OD1	2.38	0.65
1:F:33:LEU:HD23	1:F:384:PHE:O	1.95	0.65
1:D:405:PHE:O	1:D:408:PRO:HG3	1.97	0.65
1:A:143:ARG:NH2	1:A:147:GLU:HG3	2.11	0.65
1:A:167:ASN:ND2	1:A:490:SER:OG	2.30	0.65
1:D:444:LEU:HD23	2:D:501:HEM:HBC2	1.77	0.65
1:F:354:ALA:HB3	1:F:417:LEU:HD21	1.72	0.65
1:D:249:ALA:O	1:D:252:VAL:HG12	1.96	0.64
1:A:172:PHE:O	1:A:176:ARG:HB2	1.97	0.64
1:D:354:ALA:HB2	1:D:417:LEU:HD12	1.77	0.64
1:A:354:ALA:HB3	1:A:417:LEU:HD21	1.79	0.64
1:E:413:PRO:O	1:E:417:LEU:HD23	1.97	0.64
1:F:374:VAL:CG2	1:F:386:PRO:O	2.44	0.64
1:B:33:LEU:HD23	1:B:384:PHE:O	1.97	0.64
1:E:39:PRO:HG3	1:E:72:HIS:CE1	2.33	0.64
1:D:157:ILE:HD11	1:D:455:THR:HG22	1.78	0.64
1:D:374:VAL:CG2	1:D:376:LYS:O	2.45	0.64
1:E:248:ILE:O	1:E:252:VAL:HG23	1.98	0.64
1:D:39:PRO:HG3	1:D:72:HIS:ND1	2.12	0.64
1:C:104:GLN:HB3	1:C:118:PHE:HE2	1.62	0.64
1:F:42:PHE:HA	4:F:616:HOH:O	1.96	0.64
1:A:135:LEU:O	1:A:140:VAL:HB	1.97	0.64
1:D:77:ARG:NH2	1:D:386:PRO:HG2	2.12	0.64
1:A:378:THR:HG22	1:A:385:LEU:HB2	1.80	0.64
1:D:391:VAL:O	1:D:393:PRO:HD3	1.98	0.63
1:B:420:LYS:HD2	1:B:422:GLN:OE1	1.98	0.63
1:B:354:ALA:HB1	1:B:417:LEU:HD21	1.79	0.63
1:E:405:PHE:O	1:E:408:PRO:HG3	1.98	0.63
1:B:79:VAL:HG21	1:B:385:LEU:CD2	2.29	0.63
1:A:230:LEU:O	1:A:235:GLN:NE2	2.29	0.63
1:D:107:PHE:O	1:D:110:VAL:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:271:PHE:CD2	1:F:291:LEU:HB2	2.34	0.62
1:C:223:PHE:O	1:C:227:MET:HG3	1.99	0.62
1:E:128:ARG:NH1	2:E:501:HEM:O1D	2.29	0.62
1:F:156:LEU:HD13	1:F:177:THR:OG1	1.98	0.62
1:B:392:TYR:HB3	1:B:394:MET:HE3	1.81	0.62
1:A:416:PHE:O	1:A:417:LEU:HD22	1.99	0.62
1:F:170:PRO:HB2	1:F:174:LEU:HD23	1.82	0.62
1:C:330:GLU:OE1	1:C:349:MET:C	2.43	0.62
1:B:476:LYS:HB2	1:B:485:ARG:HA	1.81	0.62
1:F:107:PHE:CE2	3:F:502:SNE:H7	2.35	0.62
1:D:152:GLU:HG3	1:D:177:THR:HG23	1.82	0.61
1:A:110:VAL:HG21	1:A:241:LEU:HB3	1.81	0.61
1:C:82:CYS:SG	1:C:394:MET:HG3	2.40	0.61
1:A:275:MET:HG2	1:A:286:PHE:O	2.01	0.61
1:A:416:PHE:C	1:A:417:LEU:HD22	2.25	0.61
1:C:104:GLN:HG3	1:C:107:PHE:HD1	1.65	0.61
1:E:111:PHE:CE2	1:E:297:ASN:OD1	2.53	0.61
1:C:354:ALA:HB1	1:C:417:LEU:CD2	2.30	0.61
1:E:199:LEU:HG	1:E:203:ARG:HH21	1.65	0.61
1:C:59:MET:HE1	1:C:82:CYS:SG	2.41	0.61
1:E:73:LEU:HB2	1:E:76:ARG:HD3	1.82	0.61
1:D:259:LEU:HD12	4:D:635:HOH:O	2.01	0.61
1:C:234:GLN:OE1	1:C:234:GLN:N	2.33	0.61
1:E:257:ARG:HG3	4:E:631:HOH:O	1.99	0.61
1:E:72:HIS:HA	1:E:76:ARG:O	2.00	0.60
1:D:419:GLU:HG2	1:D:420:LYS:N	2.16	0.60
1:B:354:ALA:CB	1:B:417:LEU:CD2	2.78	0.60
1:C:413:PRO:O	1:C:417:LEU:HD23	2.01	0.60
1:E:365:VAL:O	1:E:481:ALA:HA	2.01	0.60
1:C:141:GLY:H	1:C:145:ILE:HD11	1.65	0.60
1:D:148:ARG:HA	1:D:148:ARG:HH11	1.64	0.60
1:D:466:GLN:OE1	1:D:471:ILE:HA	2.02	0.60
1:F:39:PRO:HG3	1:F:72:HIS:CE1	2.37	0.60
1:B:346:ARG:HG3	1:B:347:ALA:N	2.16	0.60
1:C:148:ARG:NH1	1:C:184:SER:OG	2.35	0.60
1:D:285:GLU:OE1	1:D:285:GLU:HA	2.01	0.59
1:E:351:TYR:O	1:E:355:VAL:HG23	2.02	0.59
1:F:495:HIS:O	1:F:495:HIS:HD2	1.84	0.59
1:B:94:GLN:HB3	1:B:97:GLU:OE2	2.02	0.59
1:E:452:PHE:O	1:E:456:VAL:HG23	2.02	0.59
1:F:346:ARG:HB2	1:F:353:GLU:OE1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:PHE:HE1	3:C:502:SNE:H1	1.66	0.59
1:B:225:SER:HA	1:B:228:LYS:CE	2.30	0.59
1:C:117:VAL:HG11	1:C:118:PHE:CE1	2.37	0.59
1:B:130:PHE:HD2	1:B:274:ARG:HH11	1.49	0.59
1:B:318:MET:SD	1:B:489:MET:HE3	2.42	0.59
1:C:303:THR:HG22	1:C:304:GLU:N	2.16	0.59
1:F:259:LEU:O	1:F:261:PRO:HD3	2.01	0.59
1:D:128:ARG:HD2	2:D:501:HEM:O1D	2.02	0.59
1:E:335:ILE:HD13	1:E:341:PRO:HB3	1.85	0.59
1:F:157:ILE:HD11	1:F:455:THR:HG22	1.85	0.59
1:B:94:GLN:HG2	1:B:97:GLU:OE2	2.02	0.59
1:C:268:ILE:HG23	1:C:291:LEU:HD11	1.84	0.59
1:D:312:TYR:CE2	1:D:484:PRO:CB	2.86	0.58
1:B:316:LEU:HD13	1:B:411:PHE:CE1	2.38	0.58
1:C:199:LEU:C	1:C:199:LEU:CD1	2.75	0.58
1:F:316:LEU:O	1:F:319:LYS:N	2.35	0.58
1:A:82:CYS:N	4:A:658:HOH:O	2.35	0.58
1:A:281:ASN:OD1	1:A:281:ASN:C	2.47	0.58
1:B:152:GLU:HG3	1:B:177:THR:HG23	1.84	0.58
1:B:174:LEU:HD12	1:B:310:LEU:HD13	1.85	0.58
1:A:143:ARG:HH21	1:A:147:GLU:HG3	1.67	0.58
1:A:61:ILE:O	1:A:64:ARG:HB3	2.04	0.58
1:A:392:TYR:HB3	1:A:394:MET:HE3	1.85	0.58
1:B:97:GLU:O	1:B:374:VAL:HA	2.04	0.58
1:F:453:PHE:O	1:F:457:MET:HG2	2.04	0.58
1:A:252:VAL:HG13	1:A:253:GLU:N	2.19	0.58
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.34	0.57
1:C:130:PHE:CE2	1:C:274:ARG:CD	2.87	0.57
1:B:148:ARG:NH2	1:B:190:ARG:HD2	2.19	0.57
1:E:110:VAL:CG1	1:E:111:PHE:CE1	2.88	0.57
1:E:312:TYR:HH	1:E:362:PHE:HE2	1.51	0.57
1:D:433:SER:CB	2:D:501:HEM:HBA1	2.34	0.57
1:D:369:SER:HB2	1:D:395:LEU:HG	1.87	0.57
1:D:354:ALA:HB2	1:D:417:LEU:HD11	1.68	0.57
1:C:322:GLU:HG3	1:C:323:VAL:HG23	1.87	0.57
1:C:107:PHE:CE2	3:C:502:SNE:H7	2.39	0.57
1:E:146:GLU:OE1	1:E:342:LYS:HG3	2.04	0.57
1:B:79:VAL:HG21	1:B:385:LEU:HD23	1.85	0.57
1:C:40:LEU:HB3	1:C:41:PRO:HD3	1.78	0.57
1:E:294:THR:O	1:E:298:LEU:HD23	2.05	0.57
1:E:374:VAL:HG23	1:E:388:GLY:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:444:LEU:HD23	2:E:501:HEM:CBC	2.35	0.56
2:D:501:HEM:HMC2	2:D:501:HEM:CBC	2.25	0.56
1:B:144:GLY:HA3	4:B:622:HOH:O	2.04	0.56
1:C:94:GLN:O	1:C:98:PHE:HD1	1.88	0.56
1:C:368:MET:HB3	1:C:394:MET:HE1	1.86	0.56
1:E:46:TYR:HD1	1:E:222:MET:HE1	1.70	0.56
1:F:346:ARG:CG	1:F:347:ALA:N	2.67	0.56
1:D:107:PHE:CE2	3:D:502:SNE:H7	2.40	0.56
1:D:374:VAL:HG11	1:D:386:PRO:O	2.06	0.56
1:C:474:SER:O	1:C:485:ARG:NE	2.39	0.56
1:E:223:PHE:O	1:E:227:MET:CG	2.44	0.56
1:E:379:LYS:HA	1:E:383:PHE:O	2.04	0.56
1:F:209:PHE:CE2	1:F:304:GLU:CB	2.79	0.56
1:F:291:LEU:O	1:F:295:THR:OG1	2.20	0.56
1:B:369:SER:HB2	1:B:395:LEU:HG	1.88	0.56
1:C:117:VAL:CG1	1:C:118:PHE:CE1	2.89	0.56
1:C:391:VAL:O	1:C:393:PRO:HD3	2.05	0.56
1:B:367:PRO:HD2	1:B:480:PHE:O	2.06	0.56
1:C:205:MET:SD	1:C:303:THR:HG21	2.46	0.56
1:C:271:PHE:CE2	1:C:291:LEU:HB2	2.41	0.56
1:C:367:PRO:HD2	1:C:480:PHE:O	2.04	0.56
1:F:495:HIS:O	1:F:495:HIS:CG	2.58	0.56
1:C:199:LEU:HD13	1:C:199:LEU:O	2.06	0.56
1:C:354:ALA:HB2	1:C:417:LEU:HD22	1.87	0.56
1:C:170:PRO:HB2	1:C:174:LEU:CD2	2.32	0.56
1:E:369:SER:HB2	1:E:395:LEU:HG	1.86	0.56
1:D:470:ASP:O	1:D:471:ILE:C	2.49	0.55
1:C:374:VAL:HG21	1:C:386:PRO:O	2.06	0.55
2:D:501:HEM:HMB1	2:D:501:HEM:CBB	2.30	0.55
1:A:199:LEU:HD13	1:C:164:GLY:O	2.06	0.55
1:C:104:GLN:HG3	1:C:104:GLN:O	2.06	0.55
1:E:235:GLN:HB2	4:E:630:HOH:O	2.05	0.55
1:B:94:GLN:CB	1:B:97:GLU:OE2	2.54	0.55
1:F:354:ALA:CB	1:F:417:LEU:HD22	2.35	0.55
1:E:76:ARG:NH2	1:E:103:GLU:HB3	2.22	0.55
1:A:232:GLY:HA2	4:A:633:HOH:O	2.07	0.55
1:C:452:PHE:O	1:C:456:VAL:HG23	2.07	0.55
1:E:110:VAL:HG11	1:E:111:PHE:CE1	2.42	0.55
1:A:433:SER:CB	2:A:502:HEM:HBA1	2.37	0.55
1:D:437:ARG:O	2:D:501:HEM:O2A	2.25	0.54
1:B:494:ARG:HB3	4:B:646:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:502:HEM:HMC2	2:A:502:HEM:CBC	2.28	0.54
1:C:40:LEU:N	1:C:40:LEU:HD22	2.22	0.54
1:C:46:TYR:HB2	1:C:222:MET:HE1	1.88	0.54
1:C:139:GLY:CA	1:C:145:ILE:CG2	2.77	0.54
1:E:201:LEU:HD12	1:E:201:LEU:N	2.22	0.54
1:B:386:PRO:HD2	1:B:389:THR:HG21	1.88	0.54
1:E:468:PRO:HA	1:E:471:ILE:HD12	1.89	0.54
1:E:39:PRO:HG3	1:E:72:HIS:ND1	2.22	0.54
1:F:34:PRO:HD3	1:F:383:PHE:HB3	1.89	0.54
1:E:170:PRO:HB2	1:E:174:LEU:CD2	2.36	0.54
1:F:369:SER:HB2	1:F:395:LEU:HG	1.89	0.54
1:D:39:PRO:CB	1:D:72:HIS:ND1	2.71	0.54
1:A:441:GLY:HA3	2:A:502:HEM:C3C	2.43	0.54
1:B:101:ARG:HG3	1:B:102:GLY:O	2.07	0.54
1:C:354:ALA:HB2	1:C:417:LEU:HD21	1.83	0.54
1:F:101:ARG:NH2	2:F:501:HEM:O2A	2.39	0.54
1:F:433:SER:CB	2:F:501:HEM:HBA1	2.38	0.54
1:D:148:ARG:HD3	1:D:184:SER:OG	2.08	0.54
1:C:109:TRP:CZ3	1:C:110:VAL:HG22	2.42	0.54
1:B:407:ASN:HB3	1:B:410:ASP:OD1	2.08	0.53
1:A:109:TRP:CH2	1:A:238:PHE:HB3	2.43	0.53
1:E:370:LEU:HD13	1:E:480:PHE:HE1	1.73	0.53
1:A:176:ARG:HG3	1:A:202:LEU:CD1	2.38	0.53
1:A:365:VAL:O	1:A:481:ALA:HA	2.07	0.53
1:F:186:VAL:HA	1:F:267:PHE:HB3	1.90	0.53
1:F:209:PHE:HZ	3:F:502:SNE:H9	1.73	0.53
1:A:101:ARG:HB3	1:A:120:ASN:OD1	2.09	0.53
1:C:420:LYS:O	1:C:422:GLN:HG3	2.08	0.53
1:E:110:VAL:HG13	1:E:111:PHE:H	1.66	0.53
1:E:402:PRO:HA	1:E:405:PHE:O	2.08	0.53
1:A:296:LEU:HD11	1:A:300:ILE:CD1	2.39	0.53
1:C:32:LYS:CG	1:C:33:LEU:H	2.18	0.53
1:C:368:MET:HB3	1:C:394:MET:CE	2.39	0.53
1:F:416:PHE:C	1:F:417:LEU:HD22	2.34	0.53
1:A:476:LYS:HB2	1:A:485:ARG:HA	1.90	0.53
1:E:157:ILE:CD1	1:E:460:PHE:HE2	2.22	0.53
1:D:176:ARG:HG2	1:D:198:PHE:CE2	2.43	0.53
1:B:186:VAL:HA	1:B:267:PHE:HB3	1.91	0.53
1:A:361:ARG:HH12	1:A:408:PRO:HA	1.73	0.53
1:E:157:ILE:HD12	1:E:460:PHE:HE2	1.74	0.53
1:E:197:GLU:O	1:E:201:LEU:CD1	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:PHE:HZ	3:C:502:SNE:C9	2.21	0.53
1:B:183:SER:OG	1:B:299:PHE:HE1	1.91	0.52
1:E:374:VAL:HG23	1:E:374:VAL:O	2.09	0.52
1:F:495:HIS:CD2	1:F:495:HIS:C	2.88	0.52
1:E:199:LEU:HD23	1:E:203:ARG:NH2	2.24	0.52
1:E:252:VAL:HG22	1:E:268:ILE:HD13	1.92	0.52
1:B:157:ILE:HD11	1:B:455:THR:HG22	1.90	0.52
1:C:358:GLU:HG3	1:C:411:PHE:CE1	2.45	0.52
1:E:107:PHE:O	1:E:111:PHE:HD1	1.92	0.52
1:E:324:GLU:O	1:E:327:VAL:HB	2.08	0.52
1:E:368:MET:HE3	4:E:628:HOH:O	2.09	0.52
1:E:432:PHE:HB3	1:E:439:CYS:HB3	1.91	0.52
1:D:56:ASN:O	1:D:60:LYS:HG2	2.10	0.52
2:F:501:HEM:HMB2	2:F:501:HEM:CBB	2.39	0.52
1:C:301:GLY:CA	3:C:502:SNE:H12	2.31	0.52
1:D:99:SER:OG	1:D:375:LYS:HE2	2.10	0.52
1:B:468:PRO:C	1:B:470:ASP:N	2.66	0.52
1:E:107:PHE:CZ	3:E:502:SNE:H7	2.44	0.52
1:A:432:PHE:O	1:A:433:SER:HB3	2.10	0.51
1:C:53:GLN:HB3	1:C:56:ASN:HB2	1.92	0.51
1:A:34:PRO:HD3	1:A:383:PHE:HB3	1.91	0.51
1:C:143:ARG:HH21	1:C:147:GLU:CG	2.23	0.51
1:C:289:LYS:O	1:C:291:LEU:N	2.44	0.51
1:E:367:PRO:HD2	1:E:480:PHE:O	2.11	0.51
1:A:101:ARG:HB3	1:A:120:ASN:ND2	2.26	0.51
1:B:323:VAL:O	1:B:327:VAL:HG23	2.11	0.51
1:C:324:GLU:O	1:C:327:VAL:HB	2.10	0.51
1:A:161:ARG:HB3	1:C:194:LYS:HD3	1.91	0.51
1:B:78:VAL:HG11	1:B:392:TYR:CD2	2.46	0.51
1:C:237:ALA:O	1:C:241:LEU:CD2	2.54	0.51
1:E:199:LEU:CD2	1:E:203:ARG:HH21	2.24	0.51
1:E:230:LEU:HD13	1:E:231:PRO:O	2.09	0.51
1:E:260:ASP:O	1:E:261:PRO:C	2.53	0.51
1:E:311:ARG:O	1:E:487:TYR:OH	2.24	0.51
1:F:209:PHE:CZ	3:F:502:SNE:H9	2.45	0.51
1:F:391:VAL:O	1:F:393:PRO:HD3	2.11	0.51
1:A:276:GLN:HG2	4:A:664:HOH:O	2.11	0.51
1:B:266:ASP:O	1:B:269:ASP:HB2	2.11	0.51
1:C:320:HIS:ND1	1:C:322:GLU:OE1	2.38	0.51
1:D:213:SER:HA	1:D:479:GLY:HA3	1.92	0.51
1:B:420:LYS:HG3	1:B:422:GLN:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:417:LEU:HA	1:E:422:GLN:O	2.11	0.51
1:E:458:GLN:O	1:E:458:GLN:HG2	2.10	0.51
1:E:464:SER:HB3	1:E:466:GLN:O	2.11	0.51
1:F:346:ARG:O	1:F:349:MET:N	2.27	0.51
1:E:416:PHE:C	1:E:417:LEU:HD22	2.35	0.51
1:E:439:CYS:HB2	2:E:501:HEM:C1A	2.45	0.51
1:B:467:SER:O	1:B:470:ASP:HB2	2.11	0.51
1:F:33:LEU:HD22	1:F:34:PRO:HD2	1.93	0.51
1:A:439:CYS:HB2	2:A:502:HEM:CHA	2.39	0.51
1:B:356:ILE:O	1:B:360:GLN:HG3	2.11	0.51
1:C:84:HIS:HA	1:C:398:VAL:HG13	1.93	0.51
1:E:235:GLN:OE1	1:E:235:GLN:HA	2.10	0.51
1:D:365:VAL:O	1:D:481:ALA:HA	2.11	0.50
1:A:199:LEU:HB2	4:A:649:HOH:O	2.11	0.50
1:A:378:THR:HG23	1:A:385:LEU:HD13	1.93	0.50
1:B:408:PRO:HD2	1:B:409:GLN:OE1	2.11	0.50
1:C:224:SER:C	1:C:226:VAL:N	2.65	0.50
1:E:275:MET:HG2	1:E:286:PHE:O	2.12	0.50
1:A:264:PRO:HG3	1:A:273:ILE:HD13	1.93	0.50
1:C:64:ARG:HD2	4:C:623:HOH:O	2.12	0.50
1:F:430:VAL:HG23	1:F:430:VAL:O	2.12	0.50
1:F:474:SER:O	1:F:485:ARG:NE	2.43	0.50
1:D:260:ASP:C	1:D:262:ASN:H	2.19	0.50
1:B:107:PHE:CE2	3:B:502:SNE:H7	2.47	0.50
1:B:315:LEU:HD13	1:B:487:TYR:CD2	2.46	0.50
1:E:222:MET:HE2	1:E:223:PHE:CZ	2.46	0.50
1:E:325:ALA:O	1:E:328:HIS:N	2.45	0.50
1:F:195:ASP:HB3	1:F:198:PHE:HB3	1.94	0.50
1:A:170:PRO:HG3	1:A:489:MET:SD	2.52	0.50
1:E:110:VAL:CG1	1:E:111:PHE:H	2.21	0.50
1:D:439:CYS:HB2	2:D:501:HEM:C1A	2.47	0.50
1:A:296:LEU:HD13	1:A:300:ILE:HG13	1.94	0.50
1:A:396:GLY:O	1:A:400:ARG:HG3	2.12	0.50
1:B:183:SER:OG	1:B:299:PHE:CE1	2.65	0.50
1:B:296:LEU:HG	1:B:300:ILE:HD11	1.93	0.50
1:E:462:LEU:HD23	1:E:489:MET:HE1	1.94	0.50
1:D:433:SER:HB3	2:D:501:HEM:HBA1	1.94	0.49
1:A:315:LEU:HB2	1:A:487:TYR:CE2	2.46	0.49
1:E:199:LEU:CG	1:E:203:ARG:HH21	2.24	0.49
1:A:169:ASP:HB3	1:C:167:ASN:HB3	1.93	0.49
1:D:186:VAL:HA	1:D:267:PHE:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:SER:CB	2:B:501:HEM:HBA1	2.42	0.49
1:A:109:TRP:CZ3	1:A:110:VAL:HG23	2.45	0.49
1:A:310:LEU:HD23	1:A:453:PHE:CE1	2.47	0.49
1:B:39:PRO:HG3	1:B:72:HIS:CE1	2.47	0.49
1:C:220:TYR:HA	1:C:227:MET:SD	2.53	0.49
1:C:288:LEU:O	1:C:289:LYS:C	2.56	0.49
1:A:412:ASN:OD1	1:A:414:GLN:HG2	2.12	0.49
1:C:369:SER:HB2	1:C:395:LEU:HG	1.94	0.49
1:C:468:PRO:O	1:C:469:LYS:C	2.55	0.49
1:E:74:GLY:HA2	1:E:223:PHE:HE2	1.77	0.49
1:C:104:GLN:CG	1:C:107:PHE:HD1	2.25	0.49
1:A:354:ALA:CB	1:A:417:LEU:HD22	2.38	0.49
1:B:301:GLY:HA2	3:B:502:SNE:H12	1.95	0.49
1:E:45:ASN:HD22	1:E:48:GLN:HE22	1.59	0.49
1:A:182:ILE:O	1:A:186:VAL:HG22	2.13	0.49
1:A:458:GLN:C	1:A:494:ARG:HH11	2.21	0.49
1:F:342:LYS:O	1:F:345:ASP:HB2	2.12	0.49
1:A:89:GLU:O	1:A:93:ASP:HB2	2.12	0.48
1:D:252:VAL:CG1	1:D:253:GLU:N	2.76	0.48
1:C:42:PHE:CD1	1:C:75:PRO:HB3	2.48	0.48
1:C:259:LEU:O	1:C:261:PRO:HD3	2.12	0.48
1:C:289:LYS:O	1:C:290:ASN:C	2.56	0.48
1:E:316:LEU:HD13	1:E:411:PHE:CE1	2.48	0.48
1:F:60:LYS:O	1:F:63:GLU:HB2	2.13	0.48
1:B:59:MET:O	1:B:62:SER:OG	2.30	0.48
1:E:271:PHE:CE2	1:E:291:LEU:HB2	2.49	0.48
1:A:407:ASN:N	1:A:408:PRO:HD3	2.28	0.48
1:D:115:GLY:O	1:D:119:SER:HB3	2.14	0.48
1:D:407:ASN:N	1:D:408:PRO:CD	2.76	0.48
1:B:468:PRO:C	1:B:470:ASP:H	2.20	0.48
1:E:396:GLY:O	1:E:400:ARG:HG3	2.14	0.48
1:A:271:PHE:CE2	1:A:291:LEU:HB2	2.49	0.48
1:A:321:PRO:O	1:A:322:GLU:C	2.57	0.48
1:B:265:ARG:CZ	4:B:610:HOH:O	2.61	0.48
1:C:244:LEU:HB3	1:C:296:LEU:HD11	1.95	0.48
1:D:193:TYR:N	4:D:633:HOH:O	2.34	0.48
1:A:184:SER:O	1:A:188:GLY:HA2	2.14	0.48
1:E:170:PRO:O	1:E:174:LEU:HD23	2.14	0.48
1:D:39:PRO:CG	1:D:72:HIS:ND1	2.76	0.48
1:B:334:VAL:O	1:B:334:VAL:CG1	2.62	0.48
1:F:333:ARG:HG2	1:F:333:ARG:HH11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:346:ARG:HG2	1:F:347:ALA:H	1.79	0.48
1:D:419:GLU:H	1:D:419:GLU:CD	2.22	0.48
1:A:259:LEU:O	1:A:261:PRO:HD3	2.14	0.48
1:F:45:ASN:OD1	1:F:72:HIS:N	2.46	0.48
2:B:501:HEM:HBC2	2:B:501:HEM:HMC2	1.96	0.47
1:C:104:GLN:O	1:C:104:GLN:CG	2.62	0.47
1:F:354:ALA:HB2	1:F:417:LEU:HD22	1.92	0.47
1:A:312:TYR:CE2	1:A:363:GLY:HA2	2.49	0.47
1:F:182:ILE:HD13	2:F:501:HEM:CBC	2.44	0.47
1:D:190:ARG:NH2	4:D:622:HOH:O	2.36	0.47
1:E:418:ASN:ND2	1:E:422:GLN:HB2	2.29	0.47
1:F:84:HIS:C	1:F:84:HIS:ND1	2.72	0.47
1:A:433:SER:C	1:A:434:ILE:HG23	2.39	0.47
1:F:365:VAL:O	1:F:481:ALA:HA	2.14	0.47
1:D:374:VAL:CG1	1:D:386:PRO:O	2.62	0.47
1:A:224:SER:O	1:A:228:LYS:HE2	2.13	0.47
1:C:114:TYR:CD1	1:C:114:TYR:N	2.82	0.47
1:C:374:VAL:HG23	1:C:388:GLY:N	2.30	0.47
1:F:302:GLY:CA	2:F:501:HEM:HBC2	2.45	0.47
1:B:269:ASP:O	1:B:270:SER:C	2.57	0.47
1:B:306:VAL:CG2	2:B:501:HEM:HAB	2.44	0.47
1:C:270:SER:HA	1:C:273:ILE:HD12	1.97	0.47
1:C:400:ARG:HA	1:C:408:PRO:HB3	1.96	0.47
1:C:460:PHE:CD1	1:C:491:PHE:HB3	2.49	0.47
1:E:78:VAL:HG11	1:E:392:TYR:CD2	2.50	0.47
1:E:444:LEU:HD23	2:E:501:HEM:HBC2	1.97	0.47
1:F:392:TYR:HB3	1:F:394:MET:CE	2.40	0.47
1:B:441:GLY:HA3	2:B:501:HEM:C3C	2.49	0.47
1:E:199:LEU:CD2	1:E:203:ARG:NH2	2.78	0.47
1:F:345:ASP:O	1:F:349:MET:HG3	2.15	0.47
1:A:74:GLY:HA3	1:A:222:MET:O	2.15	0.47
1:B:365:VAL:O	1:B:481:ALA:HA	2.15	0.47
2:B:501:HEM:HBB2	2:B:501:HEM:CMB	2.45	0.47
1:C:108:ASP:OD1	1:C:112:LYS:O	2.33	0.47
1:E:109:TRP:CE3	1:E:109:TRP:C	2.91	0.47
1:F:101:ARG:NH1	2:F:501:HEM:O2A	2.47	0.47
1:C:156:LEU:HD22	1:C:177:THR:HG21	1.97	0.46
1:E:230:LEU:HD13	1:E:231:PRO:N	2.30	0.46
1:E:370:LEU:HD13	1:E:480:PHE:CE1	2.49	0.46
1:F:315:LEU:HD13	1:F:487:TYR:CD2	2.50	0.46
1:F:322:GLU:HG2	1:F:323:VAL:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:476:LYS:HB2	1:D:485:ARG:HA	1.97	0.46
1:A:418:ASN:HB2	1:A:419:GLU:OE1	2.15	0.46
1:B:260:ASP:O	1:B:262:ASN:N	2.49	0.46
1:C:291:LEU:HD12	1:C:291:LEU:O	2.15	0.46
1:E:467:SER:O	1:E:470:ASP:N	2.48	0.46
1:D:358:GLU:HG3	1:D:411:PHE:CE1	2.50	0.46
1:A:367:PRO:HD2	1:A:480:PHE:O	2.16	0.46
1:B:321:PRO:O	1:B:322:GLU:C	2.58	0.46
1:E:53:GLN:HB3	1:E:56:ASN:HB2	1.97	0.46
1:E:201:LEU:N	1:E:201:LEU:CD1	2.78	0.46
1:F:331:ILE:HG21	1:F:458:GLN:HB2	1.96	0.46
1:F:433:SER:HB2	2:F:501:HEM:HBA1	1.96	0.46
1:D:271:PHE:CE2	1:D:291:LEU:HB2	2.51	0.46
1:A:296:LEU:HD11	1:A:300:ILE:HD11	1.95	0.46
1:B:172:PHE:O	1:B:173:PHE:C	2.59	0.46
1:E:92:VAL:HG23	1:E:434:ILE:CD1	2.38	0.46
1:E:110:VAL:CG1	1:E:111:PHE:HD1	2.20	0.46
1:A:101:ARG:HB3	1:A:120:ASN:CG	2.40	0.46
1:A:439:CYS:HA	2:A:502:HEM:C4D	2.50	0.46
1:B:402:PRO:HA	1:B:405:PHE:O	2.16	0.46
1:E:432:PHE:CZ	2:E:501:HEM:HBB2	2.51	0.46
1:F:117:VAL:HG22	2:F:501:HEM:HAD1	1.98	0.46
1:A:73:LEU:HD12	1:A:78:VAL:HG21	1.96	0.46
1:E:461:ARG:NH1	1:E:495:HIS:ND1	2.64	0.46
1:D:260:ASP:O	1:D:262:ASN:N	2.48	0.46
1:D:281:ASN:OD1	1:D:281:ASN:C	2.58	0.46
1:A:101:ARG:N	1:A:120:ASN:OD1	2.49	0.46
1:B:264:PRO:HB3	1:B:269:ASP:HB3	1.98	0.46
1:C:45:ASN:OD1	1:C:72:HIS:N	2.44	0.46
1:A:354:ALA:HB1	1:A:417:LEU:HD21	1.76	0.46
1:A:419:GLU:CD	1:A:419:GLU:H	2.23	0.46
1:B:472:ASP:OD1	1:B:474:SER:OG	2.32	0.46
1:A:101:ARG:HB3	1:A:120:ASN:HD21	1.80	0.46
1:E:346:ARG:HG3	1:E:347:ALA:N	2.30	0.46
1:F:271:PHE:HB3	1:F:291:LEU:HD13	1.97	0.46
1:A:210:GLN:NE2	4:A:672:HOH:O	2.48	0.46
1:C:40:LEU:CD1	1:C:41:PRO:HD3	2.45	0.46
1:F:252:VAL:HG13	1:F:253:GLU:N	2.31	0.46
1:B:351:TYR:O	1:B:355:VAL:HG23	2.16	0.45
1:C:406:SER:O	1:C:407:ASN:HB2	2.16	0.45
1:D:252:VAL:HG13	1:D:253:GLU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:PHE:O	1:A:80:VAL:N	2.42	0.45
1:B:77:ARG:NH2	1:B:386:PRO:HG2	2.32	0.45
1:B:373:ARG:NH1	1:B:388:GLY:O	2.49	0.45
1:C:464:SER:OG	1:C:465:SER:N	2.49	0.45
1:E:370:LEU:CD2	3:E:502:SNE:H5	2.46	0.45
1:D:50:ASN:C	1:D:50:ASN:OD1	2.59	0.45
1:D:148:ARG:HH21	1:D:190:ARG:HB3	1.81	0.45
1:A:161:ARG:O	1:A:164:GLY:N	2.49	0.45
1:A:170:PRO:O	1:A:171:THR:C	2.58	0.45
1:A:197:GLU:O	1:A:198:PHE:C	2.58	0.45
1:B:271:PHE:CE2	1:B:291:LEU:HB2	2.51	0.45
1:C:117:VAL:HG12	1:C:118:PHE:N	2.31	0.45
1:A:85:ASP:O	1:A:89:GLU:HG3	2.16	0.45
1:A:335:ILE:HD13	1:A:341:PRO:HB3	1.97	0.45
1:C:130:PHE:CD2	1:C:274:ARG:HD3	2.52	0.45
1:C:199:LEU:CD1	1:C:203:ARG:NE	2.78	0.45
1:E:46:TYR:CD1	1:E:222:MET:HE1	2.50	0.45
1:F:130:PHE:CE1	1:F:271:PHE:HD1	2.34	0.45
1:D:453:PHE:O	1:D:457:MET:HG2	2.16	0.45
1:A:130:PHE:CE1	1:A:271:PHE:HD1	2.34	0.45
1:A:379:LYS:HE2	1:A:379:LYS:HB2	1.79	0.45
1:A:433:SER:O	1:A:434:ILE:HG23	2.17	0.45
1:E:472:ASP:OD1	1:E:472:ASP:C	2.60	0.45
1:F:374:VAL:HG23	1:F:374:VAL:O	2.15	0.45
1:D:406:SER:O	1:D:407:ASN:HB2	2.17	0.45
1:A:369:SER:HB2	1:A:395:LEU:HG	1.99	0.45
1:B:468:PRO:HA	1:B:471:ILE:HG13	1.98	0.45
1:E:136:ARG:O	1:E:142:LYS:NZ	2.32	0.45
1:E:314:PHE:CD2	1:E:462:LEU:HD21	2.51	0.45
1:E:437:ARG:HE	2:E:501:HEM:CGD	2.29	0.45
1:D:304:GLU:O	1:D:308:THR:OG1	2.24	0.45
1:B:260:ASP:C	1:B:262:ASN:N	2.74	0.45
1:D:242:GLN:NE2	1:D:245:GLU:OE1	2.46	0.45
1:B:204:MET:HG2	1:B:240:LEU:HD22	1.99	0.45
1:C:145:ILE:HG13	1:C:146:GLU:N	2.32	0.45
1:C:392:TYR:HB3	1:C:394:MET:CE	2.46	0.45
1:E:460:PHE:CD1	1:E:491:PHE:HB3	2.51	0.45
1:D:312:TYR:CD2	1:D:484:PRO:CG	3.00	0.45
1:D:413:PRO:O	1:D:417:LEU:HD13	2.17	0.45
1:A:148:ARG:NH1	1:A:151:GLU:HB3	2.32	0.45
1:B:94:GLN:CG	1:B:97:GLU:OE2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ARG:NH1	2:B:501:HEM:O2A	2.40	0.45
1:C:130:PHE:CD2	1:C:274:ARG:CD	3.00	0.45
1:F:115:GLY:O	1:F:119:SER:HB3	2.17	0.45
1:A:419:GLU:HG2	1:A:420:LYS:H	1.81	0.45
1:A:419:GLU:HG2	1:A:420:LYS:N	2.32	0.45
1:C:289:LYS:O	1:C:292:VAL:N	2.50	0.45
1:E:94:GLN:O	1:E:98:PHE:HD1	1.99	0.45
1:E:152:GLU:CD	1:E:180:ASN:HD22	2.24	0.45
1:F:235:GLN:HA	1:F:235:GLN:OE1	2.16	0.45
1:B:84:HIS:HA	1:B:398:VAL:HG13	2.00	0.44
1:B:103:GLU:HG3	1:B:104:GLN:N	2.31	0.44
1:E:59:MET:CE	1:E:397:SER:HB3	2.47	0.44
1:D:148:ARG:NH2	1:D:190:ARG:HD2	2.31	0.44
1:B:174:LEU:HD13	1:B:174:LEU:HA	1.87	0.44
1:E:319:LYS:HD3	1:E:471:ILE:HB	1.99	0.44
1:E:420:LYS:HG3	1:E:422:GLN:HG3	1.99	0.44
1:A:331:ILE:HG21	1:A:458:GLN:HB2	1.99	0.44
1:A:458:GLN:C	1:A:494:ARG:NH1	2.76	0.44
1:C:115:GLY:O	1:C:119:SER:HB3	2.17	0.44
1:C:157:ILE:HD13	1:C:460:PHE:HE2	1.82	0.44
1:E:412:ASN:HA	1:E:413:PRO:HD3	1.70	0.44
1:E:429:PHE:CZ	1:E:431:PRO:HG3	2.52	0.44
1:D:315:LEU:HD13	1:D:487:TYR:CD2	2.51	0.44
1:B:242:GLN:NE2	1:B:245:GLU:OE1	2.50	0.44
3:E:502:SNE:H6	3:E:502:SNE:H1	1.16	0.44
1:F:345:ASP:O	1:F:346:ARG:C	2.61	0.44
1:A:62:SER:C	1:A:64:ARG:H	2.26	0.44
1:A:264:PRO:HB3	1:A:269:ASP:HB3	1.99	0.44
1:A:391:VAL:O	1:A:393:PRO:HD3	2.17	0.44
1:B:296:LEU:O	1:B:300:ILE:HG13	2.17	0.44
1:C:40:LEU:HD13	1:C:40:LEU:HA	1.40	0.44
1:B:89:GLU:CD	1:B:381:ARG:HH21	2.26	0.44
1:B:370:LEU:HD12	4:B:653:HOH:O	2.16	0.44
1:E:418:ASN:HD21	1:E:422:GLN:HB2	1.82	0.44
1:D:333:ARG:HH11	1:D:333:ARG:HG2	1.82	0.44
1:D:439:CYS:HB2	2:D:501:HEM:C4A	2.51	0.44
1:A:210:GLN:CD	4:A:672:HOH:O	2.60	0.44
1:A:458:GLN:O	1:A:494:ARG:NH1	2.50	0.44
1:C:39:PRO:CG	1:C:72:HIS:ND1	2.78	0.44
1:C:343:PHE:O	1:C:344:GLU:C	2.61	0.44
1:F:328:HIS:O	1:F:329:GLU:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:358:GLU:HG3	1:F:411:PHE:CD1	2.50	0.44
1:D:318:MET:SD	1:D:489:MET:HE3	2.58	0.44
1:B:35:PRO:HD2	1:B:383:PHE:CE2	2.52	0.44
1:E:220:TYR:HA	1:E:227:MET:SD	2.58	0.44
1:F:128:ARG:O	1:F:132:ILE:HG13	2.18	0.44
1:A:128:ARG:HD2	2:A:502:HEM:O1D	2.18	0.44
1:E:41:PRO:O	1:E:42:PHE:HB3	2.18	0.44
2:B:501:HEM:CBC	2:B:501:HEM:HMC2	2.48	0.43
1:D:260:ASP:C	1:D:262:ASN:N	2.76	0.43
1:A:146:GLU:O	1:A:150:GLN:HG3	2.19	0.43
1:A:186:VAL:HA	1:A:267:PHE:HB3	2.01	0.43
1:A:296:LEU:HD13	1:A:296:LEU:C	2.42	0.43
1:C:118:PHE:CD1	1:C:118:PHE:N	2.86	0.43
1:C:407:ASN:N	1:C:408:PRO:HD3	2.33	0.43
1:E:161:ARG:O	1:E:164:GLY:N	2.40	0.43
1:E:224:SER:C	1:E:226:VAL:H	2.25	0.43
1:D:345:ASP:O	1:D:349:MET:CG	2.59	0.43
1:D:432:PHE:O	1:D:433:SER:HB3	2.17	0.43
1:A:107:PHE:CZ	3:A:501:SNE:H7	2.52	0.43
1:A:437:ARG:NH1	2:A:502:HEM:O2D	2.49	0.43
1:B:100:GLY:HA3	1:B:373:ARG:HB3	2.00	0.43
1:E:272:LEU:O	1:E:275:MET:HB2	2.18	0.43
1:A:358:GLU:HG3	1:A:411:PHE:CD1	2.53	0.43
1:A:433:SER:OG	1:A:434:ILE:N	2.49	0.43
1:C:134:THR:O	1:C:135:LEU:C	2.62	0.43
1:C:311:ARG:O	1:C:487:TYR:OH	2.34	0.43
1:E:230:LEU:O	1:E:235:GLN:NE2	2.40	0.43
1:F:302:GLY:HA2	2:F:501:HEM:HBC2	2.00	0.43
1:B:272:LEU:O	1:B:275:MET:HB2	2.18	0.43
1:B:400:ARG:NH1	4:B:639:HOH:O	2.48	0.43
1:C:374:VAL:CG2	1:C:389:THR:H	2.32	0.43
1:E:230:LEU:CD2	1:E:231:PRO:HD2	2.28	0.43
1:F:472:ASP:OD1	1:F:472:ASP:C	2.60	0.43
1:C:42:PHE:CE1	1:C:75:PRO:HB3	2.54	0.43
1:D:176:ARG:HA	1:D:202:LEU:HD11	2.00	0.43
1:A:179:SER:HA	1:A:303:THR:OG1	2.18	0.43
1:C:60:LYS:HG3	1:C:64:ARG:HH21	1.83	0.43
1:E:111:PHE:O	1:E:112:LYS:C	2.59	0.43
1:F:374:VAL:HG22	1:F:389:THR:H	1.83	0.43
1:D:103:GLU:HG3	1:D:104:GLN:N	2.34	0.43
1:D:319:LYS:HD3	1:D:471:ILE:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ASP:CB	1:C:167:ASN:HB3	2.48	0.43
1:C:55:TYR:O	1:C:56:ASN:C	2.62	0.43
1:C:59:MET:CE	1:C:397:SER:HB3	2.49	0.43
1:E:172:PHE:O	1:E:173:PHE:C	2.62	0.43
1:E:181:VAL:O	1:E:184:SER:HB2	2.18	0.43
1:F:195:ASP:HB3	1:F:198:PHE:CB	2.49	0.43
1:F:205:MET:HA	1:F:208:ILE:HD12	2.00	0.43
1:A:81:LEU:CA	4:A:658:HOH:O	2.67	0.43
1:B:306:VAL:HG22	2:B:501:HEM:HAB	1.99	0.43
1:B:327:VAL:HG11	1:B:352:MET:HE1	1.93	0.43
1:F:346:ARG:HG3	1:F:347:ALA:N	2.34	0.43
1:F:474:SER:HA	1:F:475:PRO:HD3	1.92	0.43
1:B:46:TYR:HA	1:B:222:MET:HE1	2.00	0.43
1:B:432:PHE:O	1:B:433:SER:HB3	2.19	0.43
1:C:139:GLY:C	1:C:145:ILE:HG21	2.43	0.43
1:D:223:PHE:O	1:D:227:MET:SD	2.77	0.42
1:A:45:ASN:O	1:A:46:TYR:C	2.62	0.42
1:A:252:VAL:CG1	1:A:253:GLU:N	2.82	0.42
1:A:296:LEU:CD1	1:A:300:ILE:CD1	2.97	0.42
1:A:433:SER:HB2	2:A:502:HEM:HBA1	2.00	0.42
1:B:260:ASP:C	1:B:262:ASN:H	2.27	0.42
1:F:174:LEU:HD12	1:F:310:LEU:HD13	2.01	0.42
1:F:209:PHE:CD2	1:F:304:GLU:HB3	2.49	0.42
1:C:271:PHE:CG	1:C:291:LEU:HD13	2.54	0.42
1:C:335:ILE:HD13	1:C:341:PRO:HB3	2.01	0.42
1:E:458:GLN:O	1:E:458:GLN:CG	2.67	0.42
1:F:209:PHE:HE2	1:F:304:GLU:HB3	1.66	0.42
1:F:313:GLY:HA3	1:F:453:PHE:HZ	1.84	0.42
1:B:145:ILE:HD12	1:B:145:ILE:HA	1.85	0.42
1:B:302:GLY:HA2	2:B:501:HEM:C2C	2.54	0.42
1:C:439:CYS:HB2	2:C:501:HEM:C4A	2.51	0.42
1:C:468:PRO:C	1:C:470:ASP:N	2.77	0.42
1:F:170:PRO:O	1:F:171:THR:C	2.63	0.42
1:D:392:TYR:HB3	1:D:394:MET:HE3	2.01	0.42
1:A:372:ARG:NH1	4:A:606:HOH:O	2.50	0.42
1:C:139:GLY:O	1:C:145:ILE:CG1	2.62	0.42
1:E:312:TYR:HD1	1:E:312:TYR:O	2.02	0.42
1:A:135:LEU:C	1:A:140:VAL:HB	2.45	0.42
1:A:281:ASN:HA	1:A:282:PRO:HD3	1.91	0.42
1:B:439:CYS:HB2	2:B:501:HEM:C4A	2.48	0.42
1:C:402:PRO:HA	1:C:405:PHE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:HIS:ND1	1:E:84:HIS:C	2.77	0.42
1:E:224:SER:HB3	4:E:608:HOH:O	2.19	0.42
1:E:312:TYR:OH	1:E:362:PHE:HE2	2.02	0.42
1:A:148:ARG:HH12	1:A:151:GLU:HB3	1.85	0.42
1:B:416:PHE:C	1:B:417:LEU:HD22	2.45	0.42
1:C:455:THR:O	1:C:456:VAL:C	2.61	0.42
1:F:54:MET:O	1:F:55:TYR:C	2.62	0.42
1:D:116:VAL:HG12	1:D:294:THR:HG23	1.99	0.42
1:B:134:THR:O	1:B:135:LEU:C	2.60	0.42
1:E:45:ASN:HD22	1:E:48:GLN:NE2	2.18	0.42
1:E:109:TRP:O	1:E:109:TRP:CG	2.72	0.42
1:E:316:LEU:HD13	1:E:411:PHE:CD1	2.54	0.42
1:F:364:ASP:O	1:F:482:THR:OG1	2.33	0.42
1:F:368:MET:HB3	1:F:394:MET:HE1	2.01	0.42
1:A:427:ASP:HA	4:A:637:HOH:O	2.19	0.42
1:B:345:ASP:O	1:B:346:ARG:C	2.62	0.42
1:C:361:ARG:HG3	1:C:399:LEU:HB3	2.01	0.42
1:E:73:LEU:HB2	1:E:76:ARG:CD	2.48	0.42
1:E:74:GLY:CA	1:E:223:PHE:HE2	2.33	0.42
1:E:263:SER:HA	1:E:264:PRO:HD3	1.88	0.42
1:F:432:PHE:HB3	1:F:439:CYS:HB3	2.01	0.42
1:A:271:PHE:CD2	1:A:291:LEU:HB2	2.55	0.42
1:A:466:GLN:NE2	4:A:638:HOH:O	2.52	0.42
1:B:418:ASN:HD21	1:B:422:GLN:HB2	1.84	0.42
1:C:143:ARG:HH21	1:C:147:GLU:HG2	1.84	0.42
1:C:355:VAL:O	1:C:359:ILE:HG13	2.19	0.42
1:A:173:PHE:CE1	1:C:166:ALA:CB	3.02	0.42
1:B:190:ARG:HG3	1:B:190:ARG:HH11	1.84	0.42
1:B:476:LYS:N	1:B:483:ILE:O	2.51	0.42
1:F:45:ASN:O	1:F:46:TYR:C	2.63	0.42
1:F:220:TYR:HA	1:F:227:MET:SD	2.60	0.42
1:D:156:LEU:HD13	1:D:177:THR:OG1	2.20	0.41
1:D:312:TYR:HD2	1:D:484:PRO:CG	2.33	0.41
1:A:84:HIS:ND1	1:A:85:ASP:OD1	2.53	0.41
1:A:222:MET:HE2	1:A:222:MET:HB3	1.89	0.41
1:C:107:PHE:HB3	1:C:111:PHE:HE1	1.85	0.41
1:C:182:ILE:HG12	1:C:298:LEU:O	2.19	0.41
1:C:313:GLY:HA2	1:C:359:ILE:HD13	2.02	0.41
1:E:156:LEU:HD13	1:E:177:THR:OG1	2.20	0.41
1:B:228:LYS:HG3	1:B:229:HIS:CE1	2.54	0.41
1:B:305:THR:OG1	1:B:306:VAL:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:LEU:O	1:C:235:GLN:NE2	2.38	0.41
1:C:365:VAL:O	1:C:481:ALA:HA	2.20	0.41
1:E:59:MET:HE3	1:E:397:SER:HB3	2.01	0.41
1:F:224:SER:OG	1:F:225:SER:N	2.52	0.41
1:A:419:GLU:C	1:A:421:GLY:H	2.28	0.41
1:C:60:LYS:HG3	1:C:64:ARG:NH2	2.36	0.41
1:E:439:CYS:HB2	2:E:501:HEM:C4A	2.51	0.41
1:D:330:GLU:HG3	1:D:333:ARG:NH2	2.36	0.41
1:A:176:ARG:HA	1:A:202:LEU:HD11	2.01	0.41
1:A:354:ALA:HB2	1:A:417:LEU:CD2	2.49	0.41
1:B:34:PRO:HB3	1:B:68:VAL:O	2.20	0.41
1:C:40:LEU:N	1:C:40:LEU:CD2	2.83	0.41
1:C:49:LEU:HD23	1:C:57:SER:HB3	2.01	0.41
1:C:105:ALA:O	1:C:106:THR:C	2.63	0.41
1:C:123:ARG:HG3	1:C:285:GLU:OE2	2.20	0.41
1:C:252:VAL:HG23	1:C:268:ILE:CG2	2.51	0.41
1:E:137:ASP:C	1:E:139:GLY:H	2.29	0.41
1:E:319:LYS:HD2	1:E:468:PRO:O	2.19	0.41
1:F:33:LEU:CD2	1:F:34:PRO:HD2	2.51	0.41
1:A:340:GLN:HA	1:A:341:PRO:HD3	1.87	0.41
1:C:272:LEU:O	1:C:275:MET:N	2.54	0.41
1:C:340:GLN:HA	1:C:341:PRO:HD3	1.90	0.41
1:E:76:ARG:NH2	1:E:390:GLU:CD	2.79	0.41
1:E:84:HIS:HA	1:E:398:VAL:HG13	2.02	0.41
1:E:112:LYS:HB2	1:E:114:TYR:CD1	2.56	0.41
1:B:53:GLN:HB3	1:B:56:ASN:HB2	2.02	0.41
1:B:111:PHE:O	1:B:112:LYS:C	2.63	0.41
1:B:190:ARG:HG3	1:B:190:ARG:NH1	2.35	0.41
1:C:201:LEU:O	1:C:202:LEU:C	2.63	0.41
1:C:468:PRO:O	1:C:470:ASP:N	2.53	0.41
1:E:157:ILE:HD12	1:E:460:PHE:CE2	2.52	0.41
1:F:38:THR:HA	1:F:39:PRO:HD3	1.83	0.41
1:F:204:MET:HA	1:F:240:LEU:HD22	2.01	0.41
1:C:152:GLU:HG3	1:C:177:THR:HG23	2.02	0.41
1:C:260:ASP:HB3	1:C:263:SER:O	2.21	0.41
1:E:37:PRO:HB2	1:E:48:GLN:CD	2.42	0.41
1:E:199:LEU:HD23	1:E:203:ARG:HH21	1.85	0.41
1:E:418:ASN:OD1	1:E:418:ASN:C	2.63	0.41
1:F:210:GLN:O	1:F:214:THR:HG23	2.21	0.41
1:A:271:PHE:CE1	1:A:286:PHE:CD1	3.09	0.41
1:A:492:LEU:HA	1:A:493:PRO:HD2	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224:SER:C	1:E:226:VAL:N	2.78	0.41
1:E:321:PRO:HA	1:E:324:GLU:HB3	2.02	0.41
1:D:204:MET:HA	1:D:240:LEU:HD22	2.03	0.41
1:A:346:ARG:HG3	1:A:347:ALA:N	2.36	0.41
1:B:204:MET:O	1:B:205:MET:C	2.63	0.41
1:B:312:TYR:CE1	1:B:363:GLY:HA2	2.56	0.41
1:B:370:LEU:HD12	1:B:370:LEU:HA	1.76	0.41
1:B:494:ARG:O	1:B:495:HIS:HB2	2.20	0.41
1:C:201:LEU:HA	1:C:204:MET:HE3	2.03	0.41
1:F:252:VAL:CG1	1:F:253:GLU:N	2.83	0.41
1:F:281:ASN:HA	1:F:282:PRO:HD3	1.97	0.41
1:D:312:TYR:CE2	1:D:484:PRO:CA	3.04	0.41
1:D:331:ILE:HG12	1:D:349:MET:HE1	2.02	0.41
1:A:406:SER:O	1:A:407:ASN:HB2	2.20	0.41
1:A:412:ASN:HA	1:A:413:PRO:HD3	1.93	0.41
1:A:439:CYS:HA	2:A:502:HEM:CHA	2.51	0.41
1:B:272:LEU:HD23	1:B:272:LEU:HA	1.87	0.41
1:C:208:ILE:HG12	1:C:241:LEU:CD2	2.45	0.41
1:E:101:ARG:NH1	2:E:501:HEM:O2A	2.53	0.41
1:D:192:ASP:CA	4:D:633:HOH:O	2.48	0.40
1:D:225:SER:HA	1:D:228:LYS:HE3	2.02	0.40
1:D:495:HIS:HE1	4:D:646:HOH:O	2.03	0.40
1:B:117:VAL:HG22	2:B:501:HEM:HAD1	2.04	0.40
1:E:433:SER:OG	1:E:434:ILE:N	2.54	0.40
1:E:170:PRO:O	1:E:171:THR:C	2.64	0.40
1:F:39:PRO:HG3	1:F:72:HIS:ND1	2.35	0.40
1:D:324:GLU:O	1:D:327:VAL:HB	2.21	0.40
1:A:316:LEU:HD11	1:A:362:PHE:CD2	2.56	0.40
1:B:328:HIS:NE2	1:B:457:MET:HE3	2.37	0.40
1:C:55:TYR:CD2	1:C:55:TYR:C	2.99	0.40
1:E:318:MET:SD	1:E:489:MET:HE3	2.61	0.40
1:D:466:GLN:HB2	4:D:642:HOH:O	2.21	0.40
1:A:111:PHE:CE2	1:A:297:ASN:ND2	2.89	0.40
1:C:40:LEU:O	1:C:42:PHE:N	2.54	0.40
1:C:330:GLU:OE1	1:C:349:MET:HB3	2.21	0.40
1:C:348:LYS:C	1:C:350:PRO:CD	2.94	0.40
1:E:90:ALA:O	1:E:98:PHE:CD1	2.74	0.40
1:F:271:PHE:CD2	1:F:291:LEU:HD13	2.57	0.40
1:F:319:LYS:HD3	1:F:471:ILE:HB	2.03	0.40
1:A:152:GLU:HG3	1:A:177:THR:HG23	2.03	0.40
2:B:501:HEM:CBC	2:B:501:HEM:CMC	2.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:GLN:HA	1:C:414:GLN:OE1	2.22	0.40
1:C:418:ASN:OD1	1:C:420:LYS:N	2.54	0.40
1:F:368:MET:HB3	1:F:394:MET:CE	2.51	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	462/476 (97%)	408 (88%)	54 (12%)	0	100	100
1	B	463/476 (97%)	405 (88%)	58 (12%)	0	100	100
1	C	462/476 (97%)	407 (88%)	55 (12%)	0	100	100
1	D	463/476 (97%)	423 (91%)	40 (9%)	0	100	100
1	E	463/476 (97%)	395 (85%)	68 (15%)	0	100	100
1	F	463/476 (97%)	410 (89%)	53 (11%)	0	100	100
All	All	2776/2856 (97%)	2448 (88%)	328 (12%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	394/422 (93%)	383 (97%)	11 (3%)	38	64
1	B	393/422 (93%)	391 (100%)	2 (0%)	81	91
1	C	371/422 (88%)	364 (98%)	7 (2%)	50	74
1	D	392/422 (93%)	385 (98%)	7 (2%)	51	75
1	E	376/422 (89%)	368 (98%)	8 (2%)	47	72
1	F	369/422 (87%)	360 (98%)	9 (2%)	43	69
All	All	2295/2532 (91%)	2251 (98%)	44 (2%)	50	74

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	80	VAL
1	D	145	ILE
1	D	199	LEU
1	D	216	THR
1	D	285	GLU
1	D	353	GLU
1	D	486	ASN
1	A	92	VAL
1	A	97	GLU
1	A	110	VAL
1	A	116	VAL
1	A	145	ILE
1	A	273	ILE
1	A	295	THR
1	A	296	LEU
1	A	312	TYR
1	A	375	LYS
1	A	412	ASN
1	B	236	GLN
1	B	312	TYR
1	C	87	VAL
1	C	116	VAL
1	C	122	GLU
1	C	199	LEU
1	C	206	LEU
1	C	303	THR
1	C	374	VAL
1	E	47	LEU
1	E	147	GLU
1	E	206	LEU

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Mol	Chain	Res	Type
1	E	280	LYS
1	E	353	GLU
1	E	389	THR
1	E	412	ASN
1	E	434	ILE
1	F	40	LEU
1	F	80	VAL
1	F	145	ILE
1	F	161	ARG
1	F	167	ASN
1	F	199	LEU
1	F	230	LEU
1	F	468	PRO
1	F	486	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	235	GLN
1	D	360	GLN
1	A	126	GLN
1	A	167	ASN
1	A	255	ASN
1	A	297	ASN
1	B	229	HIS
1	B	466	GLN
1	C	360	GLN
1	C	477	HIS
1	E	167	ASN
1	E	254	HIS
1	E	255	ASN
1	E	328	HIS
1	E	357	HIS
1	E	477	HIS
1	F	236	GLN
1	F	466	GLN
1	F	495	HIS

5.3.3 RNA ⓘ

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](#)

12 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
3	SNE	C	502	-	10,11,11	0.62	0	10,18,18	3.20	5 (50%)
3	SNE	B	502	-	10,11,11	0.61	0	10,18,18	3.20	5 (50%)
2	HEM	F	501	1	50,50,50	1.91	9 (18%)	67,82,82	1.32	5 (7%)
3	SNE	E	502	-	10,11,11	4.08	1 (10%)	10,18,18	13.26	5 (50%)
2	HEM	D	501	1	50,50,50	1.90	8 (16%)	67,82,82	1.32	5 (7%)
2	HEM	B	501	1	50,50,50	1.91	9 (18%)	67,82,82	1.31	5 (7%)
2	HEM	E	501	1	50,50,50	1.90	8 (16%)	67,82,82	1.31	5 (7%)
3	SNE	D	502	-	10,11,11	0.62	0	10,18,18	3.20	5 (50%)
3	SNE	A	501	-	10,11,11	0.61	0	10,18,18	3.19	5 (50%)
3	SNE	F	502	-	10,11,11	0.62	0	10,18,18	3.19	5 (50%)
2	HEM	C	501	1	50,50,50	1.91	10 (20%)	67,82,82	1.31	5 (7%)
2	HEM	A	502	1	50,50,50	1.91	8 (16%)	67,82,82	1.31	5 (7%)

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
3	SNE	C	502	-	-	3/6/24/24	0/2/2/2
3	SNE	B	502	-	-	3/6/24/24	0/2/2/2
2	HEM	F	501	1	-	5/14/54/54	-
3	SNE	E	502	-	-	2/6/24/24	0/2/2/2
2	HEM	D	501	1	-	3/14/54/54	-
2	HEM	B	501	1	-	2/14/54/54	-
2	HEM	E	501	1	-	6/14/54/54	-
3	SNE	D	502	-	-	2/6/24/24	0/2/2/2
3	SNE	A	501	-	-	2/6/24/24	0/2/2/2
3	SNE	F	502	-	-	2/6/24/24	0/2/2/2
2	HEM	C	501	1	-	6/14/54/54	-
2	HEM	A	502	1	-	4/14/54/54	-

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	502	SNE	C6-C1	12.76	1.58	1.32
2	D	501	HEM	C3D-C2D	7.96	1.53	1.36
2	B	501	HEM	C3D-C2D	7.96	1.53	1.36
2	E	501	HEM	C3D-C2D	7.95	1.53	1.36
2	A	502	HEM	C3D-C2D	7.95	1.53	1.36
2	F	501	HEM	C3D-C2D	7.94	1.53	1.36
2	C	501	HEM	C3D-C2D	7.93	1.53	1.36
2	B	501	HEM	FE-ND	4.55	2.08	1.94
2	A	502	HEM	FE-ND	4.53	2.08	1.94
2	E	501	HEM	FE-ND	4.51	2.08	1.94
2	C	501	HEM	FE-ND	4.51	2.08	1.94
2	F	501	HEM	FE-ND	4.51	2.08	1.94
2	D	501	HEM	FE-ND	4.50	2.08	1.94
2	A	502	HEM	FE-NB	4.12	2.07	1.94
2	B	501	HEM	FE-NB	4.10	2.07	1.94
2	F	501	HEM	FE-NB	4.10	2.07	1.94
2	E	501	HEM	FE-NB	4.09	2.07	1.94
2	D	501	HEM	FE-NB	4.09	2.07	1.94
2	C	501	HEM	FE-NB	4.07	2.07	1.94
2	E	501	HEM	FE-NC	3.54	2.06	1.95
2	C	501	HEM	FE-NC	3.54	2.06	1.95
2	B	501	HEM	FE-NC	3.53	2.06	1.95
2	D	501	HEM	FE-NC	3.52	2.06	1.95
2	F	501	HEM	FE-NC	3.51	2.06	1.95
2	F	501	HEM	FE-NA	3.51	2.06	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	HEM	FE-NC	3.51	2.06	1.95
2	C	501	HEM	FE-NA	3.51	2.06	1.95
2	B	501	HEM	FE-NA	3.51	2.06	1.95
2	A	502	HEM	FE-NA	3.49	2.06	1.95
2	E	501	HEM	FE-NA	3.48	2.06	1.95
2	D	501	HEM	FE-NA	3.46	2.06	1.95
2	A	502	HEM	CAC-C3C	2.81	1.54	1.47
2	F	501	HEM	CAC-C3C	2.81	1.54	1.47
2	C	501	HEM	CAC-C3C	2.81	1.54	1.47
2	A	502	HEM	CAB-C3B	2.80	1.54	1.47
2	B	501	HEM	CAB-C3B	2.80	1.54	1.47
2	D	501	HEM	CAC-C3C	2.80	1.54	1.47
2	F	501	HEM	CAB-C3B	2.80	1.54	1.47
2	E	501	HEM	CAB-C3B	2.80	1.54	1.47
2	B	501	HEM	CAC-C3C	2.79	1.54	1.47
2	D	501	HEM	CAB-C3B	2.79	1.54	1.47
2	E	501	HEM	CAC-C3C	2.79	1.54	1.47
2	C	501	HEM	CAB-C3B	2.78	1.54	1.47
2	C	501	HEM	CMD-C2D	2.03	1.54	1.50
2	F	501	HEM	CMC-C2C	2.02	1.54	1.50
2	B	501	HEM	CMD-C2D	2.01	1.54	1.50
2	C	501	HEM	CMA-C3A	2.01	1.54	1.50
2	E	501	HEM	CMD-C2D	2.01	1.54	1.50
2	C	501	HEM	CMC-C2C	2.01	1.54	1.50
2	B	501	HEM	CMC-C2C	2.01	1.54	1.50
2	D	501	HEM	CMD-C2D	2.01	1.54	1.50
2	F	501	HEM	CMD-C2D	2.01	1.54	1.50
2	A	502	HEM	CMD-C2D	2.00	1.54	1.50

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	502	SNE	C7-C1-C6	-30.86	88.83	126.06
3	E	502	SNE	C4-C1-C6	-26.87	98.33	125.56
3	B	502	SNE	C4-C1-C7	6.21	115.07	108.25
3	C	502	SNE	C4-C1-C7	6.21	115.06	108.25
3	A	501	SNE	C4-C1-C7	6.21	115.06	108.25
3	D	502	SNE	C4-C1-C7	6.18	115.04	108.25
3	F	502	SNE	C4-C1-C7	6.18	115.03	108.25
3	E	502	SNE	C4-C1-C7	6.16	115.01	108.25
3	C	502	SNE	C9-C7-C1	-5.89	110.01	117.90
3	F	502	SNE	C9-C7-C1	-5.87	110.03	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	SNE	C9-C7-C1	-5.87	110.04	117.90
3	B	502	SNE	C9-C7-C1	-5.85	110.06	117.90
3	E	502	SNE	C9-C7-C1	-5.84	110.08	117.90
3	A	501	SNE	C9-C7-C1	-5.82	110.11	117.90
2	D	501	HEM	C4D-ND-C1D	5.51	111.74	105.21
2	B	501	HEM	C4D-ND-C1D	5.51	111.73	105.21
2	F	501	HEM	C4D-ND-C1D	5.50	111.72	105.21
2	A	502	HEM	C4D-ND-C1D	5.48	111.69	105.21
2	E	501	HEM	C4D-ND-C1D	5.47	111.69	105.21
2	C	501	HEM	C4D-ND-C1D	5.47	111.68	105.21
3	D	502	SNE	C4-C1-C6	-3.06	122.46	125.56
3	A	501	SNE	C4-C1-C6	-3.05	122.47	125.56
3	F	502	SNE	C4-C1-C6	-3.03	122.49	125.56
3	B	502	SNE	C4-C1-C6	-3.02	122.50	125.56
3	C	502	SNE	C7-C1-C6	-3.02	122.41	126.06
3	B	502	SNE	C7-C1-C6	-3.00	122.44	126.06
3	C	502	SNE	C4-C1-C6	-2.99	122.53	125.56
3	A	501	SNE	C7-C1-C6	-2.98	122.47	126.06
3	F	502	SNE	C7-C1-C6	-2.97	122.47	126.06
3	D	502	SNE	C7-C1-C6	-2.94	122.50	126.06
3	A	501	SNE	C3-C8-C9	2.90	116.89	114.64
3	E	502	SNE	C3-C8-C9	2.86	116.86	114.64
3	B	502	SNE	C3-C8-C9	2.86	116.85	114.64
3	F	502	SNE	C3-C8-C9	2.85	116.84	114.64
3	D	502	SNE	C3-C8-C9	2.84	116.84	114.64
3	C	502	SNE	C3-C8-C9	2.84	116.84	114.64
2	F	501	HEM	C1B-NB-C4B	2.34	107.98	105.21
2	E	501	HEM	C3B-C2B-C1B	2.33	108.16	106.41
2	C	501	HEM	C3B-C2B-C1B	2.33	108.16	106.41
2	C	501	HEM	C1B-NB-C4B	2.32	107.95	105.21
2	D	501	HEM	C1B-NB-C4B	2.31	107.94	105.21
2	A	502	HEM	C1B-NB-C4B	2.30	107.92	105.21
2	D	501	HEM	C3B-C2B-C1B	2.29	108.13	106.41
2	E	501	HEM	C1B-NB-C4B	2.29	107.92	105.21
2	B	501	HEM	C3B-C2B-C1B	2.28	108.13	106.41
2	F	501	HEM	C3B-C4B-NB	-2.28	107.83	109.47
2	F	501	HEM	C3B-C2B-C1B	2.28	108.12	106.41
2	B	501	HEM	C1B-NB-C4B	2.26	107.89	105.21
2	A	502	HEM	C3B-C2B-C1B	2.26	108.11	106.41
2	E	501	HEM	C3B-C4B-NB	-2.21	107.88	109.47
2	D	501	HEM	C3B-C4B-NB	-2.20	107.89	109.47
2	A	502	HEM	C3B-C4B-NB	-2.18	107.90	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	C3B-C4B-NB	-2.15	107.92	109.47
2	B	501	HEM	C3B-C4B-NB	-2.13	107.94	109.47
2	B	501	HEM	C2A-C1A-NA	-2.05	107.88	110.15
2	D	501	HEM	C2A-C1A-NA	-2.03	107.90	110.15
2	F	501	HEM	C2A-C1A-NA	-2.02	107.91	110.15
2	C	501	HEM	C2A-C1A-NA	-2.02	107.91	110.15
2	E	501	HEM	C2A-C1A-NA	-2.01	107.92	110.15
2	A	502	HEM	C2A-C1A-NA	-2.01	107.93	110.15

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	502	SNE	C-C2-C8-C7
3	D	502	SNE	C5-C2-C8-C7
3	A	501	SNE	C-C2-C8-C7
3	A	501	SNE	C5-C2-C8-C7
3	E	502	SNE	C-C2-C8-C7
3	E	502	SNE	C5-C2-C8-C7
3	F	502	SNE	C-C2-C8-C7
3	F	502	SNE	C5-C2-C8-C7
3	C	502	SNE	C5-C2-C8-C9
3	C	502	SNE	C-C2-C8-C9
2	A	502	HEM	C2B-C3B-CAB-CBB
2	C	501	HEM	C2B-C3B-CAB-CBB
2	E	501	HEM	C2B-C3B-CAB-CBB
3	B	502	SNE	C5-C2-C8-C9
2	C	501	HEM	C2C-C3C-CAC-CBC
3	C	502	SNE	C-C2-C8-C7
2	C	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4C-C3C-CAC-CBC
2	E	501	HEM	C4B-C3B-CAB-CBB
3	B	502	SNE	C-C2-C8-C3
2	C	501	HEM	CAA-CBA-CGA-O1A
2	E	501	HEM	CAA-CBA-CGA-O2A
2	F	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	CAA-CBA-CGA-O1A
2	A	502	HEM	CAA-CBA-CGA-O1A
2	E	501	HEM	CAA-CBA-CGA-O1A
2	A	502	HEM	CAA-CBA-CGA-O2A
2	F	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAA-CBA-CGA-O2A

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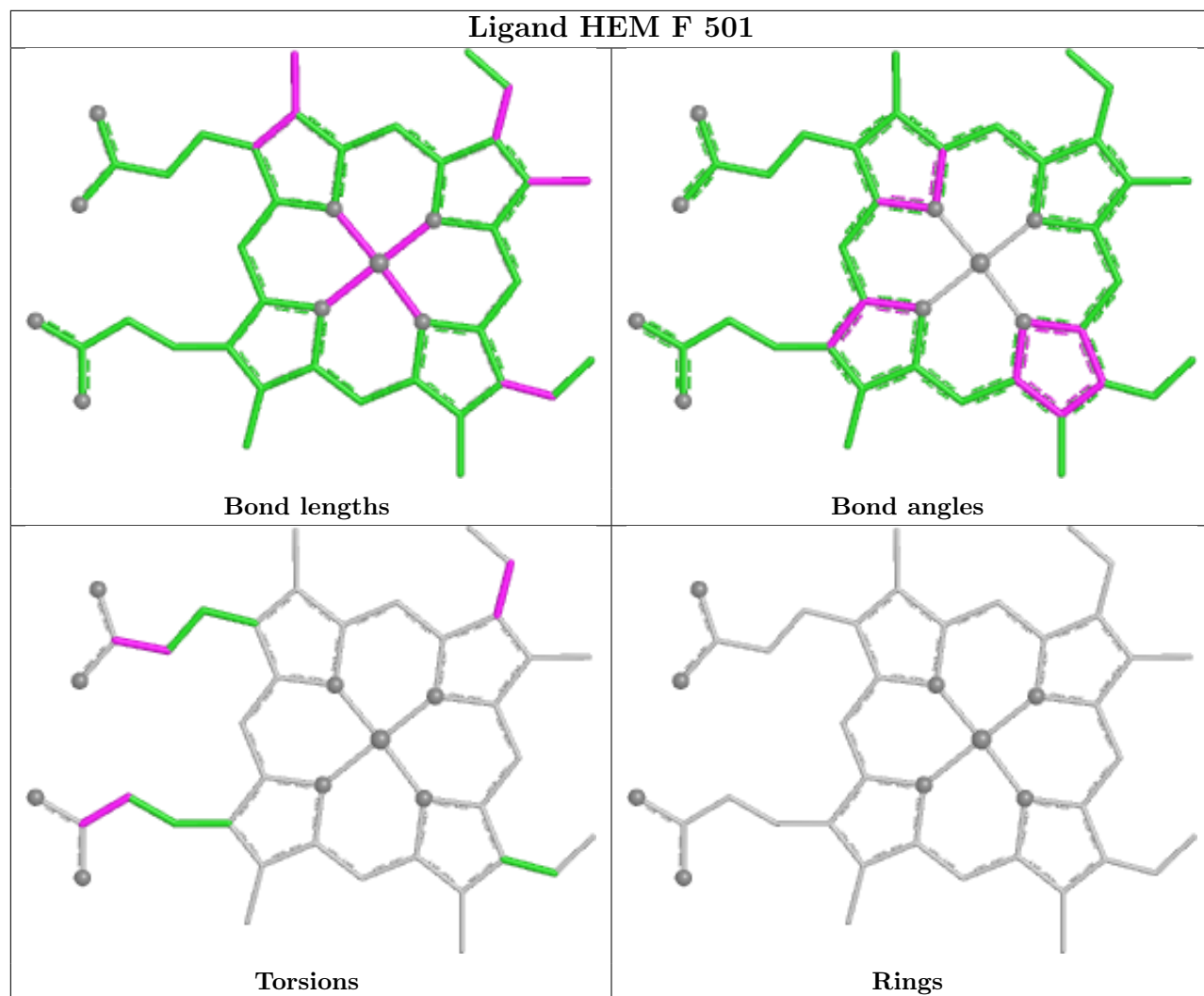
Mol	Chain	Res	Type	Atoms
2	C	501	HEM	CAA-CBA-CGA-O2A
2	A	502	HEM	C4B-C3B-CAB-CBB
2	F	501	HEM	C4C-C3C-CAC-CBC
2	E	501	HEM	CAD-CBD-CGD-O1D
2	D	501	HEM	CAA-CBA-CGA-O1A
2	D	501	HEM	CAA-CBA-CGA-O2A
3	B	502	SNE	C5-C2-C8-C3
2	E	501	HEM	CAD-CBD-CGD-O2D
2	D	501	HEM	CAD-CBD-CGD-O2D
2	F	501	HEM	CAD-CBD-CGD-O2D
2	F	501	HEM	C2C-C3C-CAC-CBC

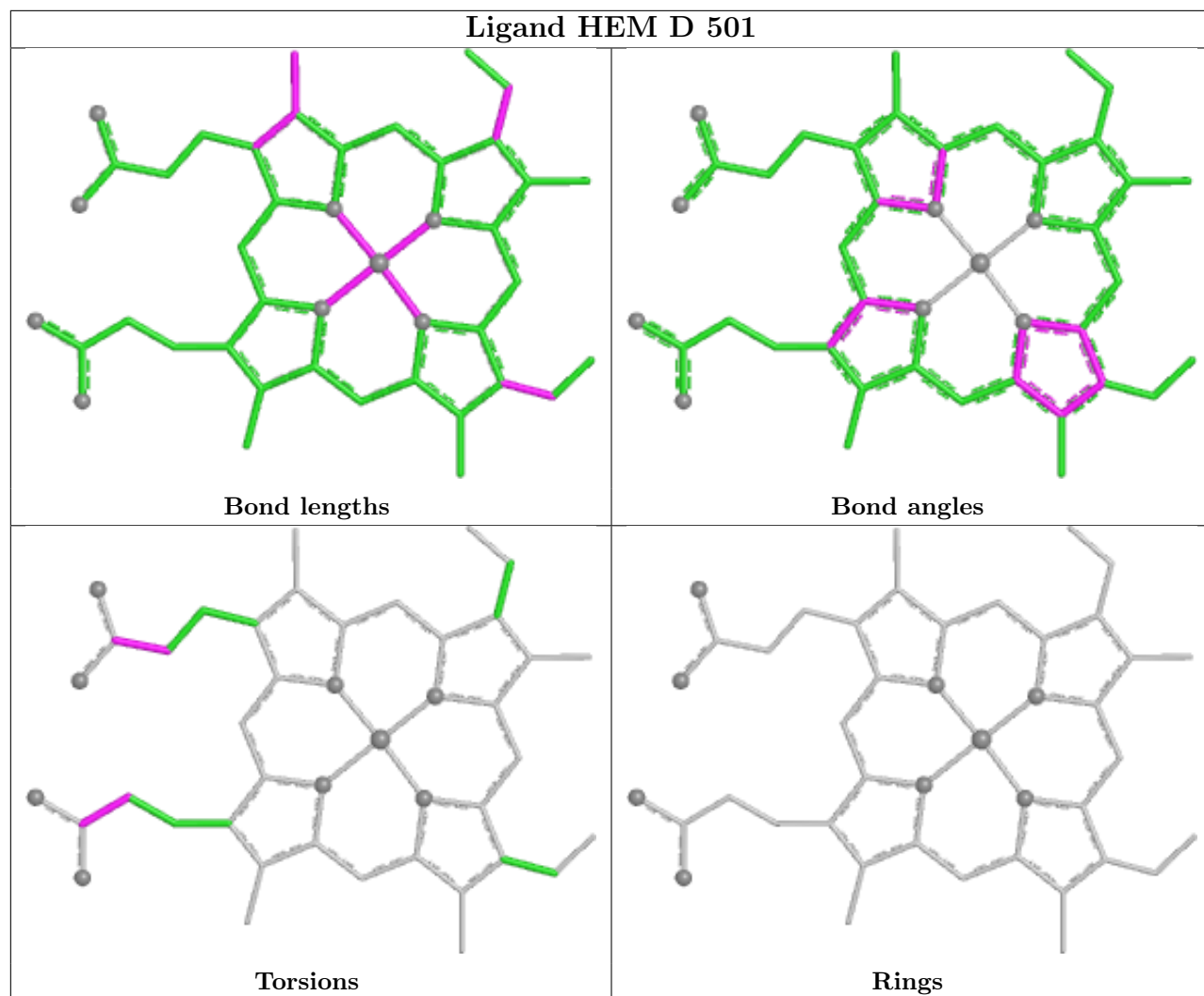
There are no ring outliers.

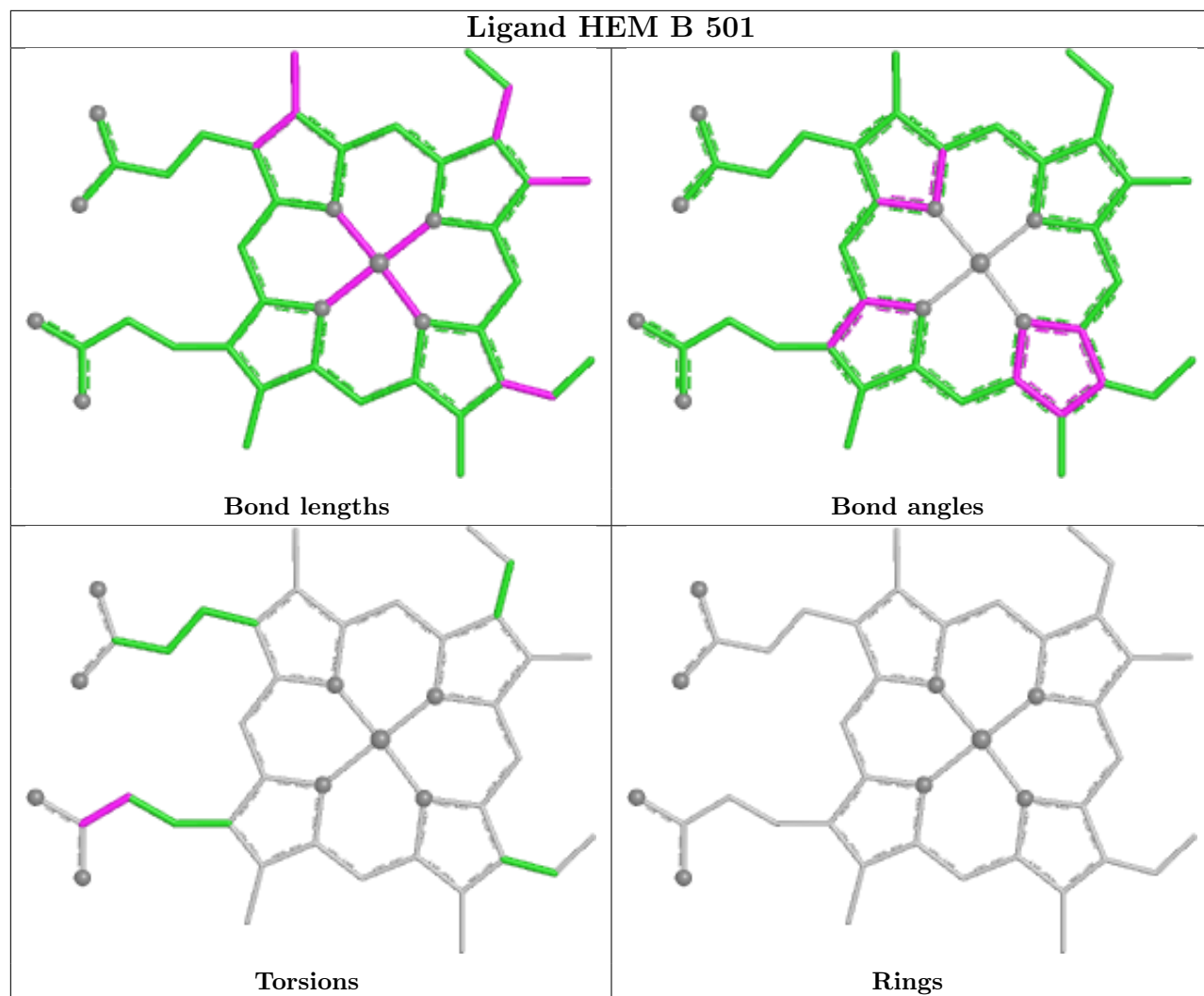
12 monomers are involved in 87 short contacts:

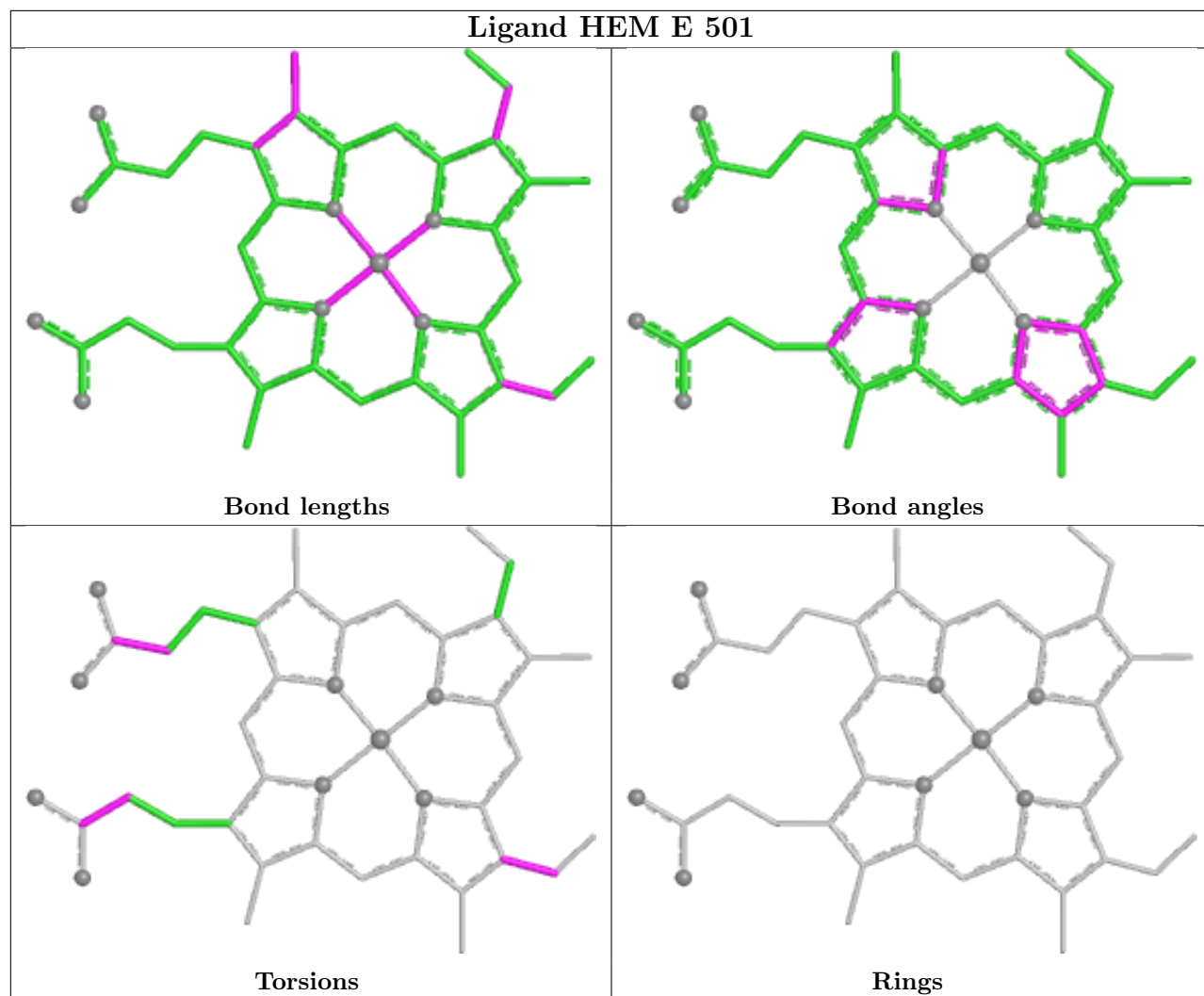
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	SNE	6	0
3	B	502	SNE	2	0
2	F	501	HEM	13	0
3	E	502	SNE	4	0
2	D	501	HEM	15	0
2	B	501	HEM	17	0
2	E	501	HEM	10	0
3	D	502	SNE	1	0
3	A	501	SNE	1	0
3	F	502	SNE	3	0
2	C	501	HEM	3	0
2	A	502	HEM	12	0

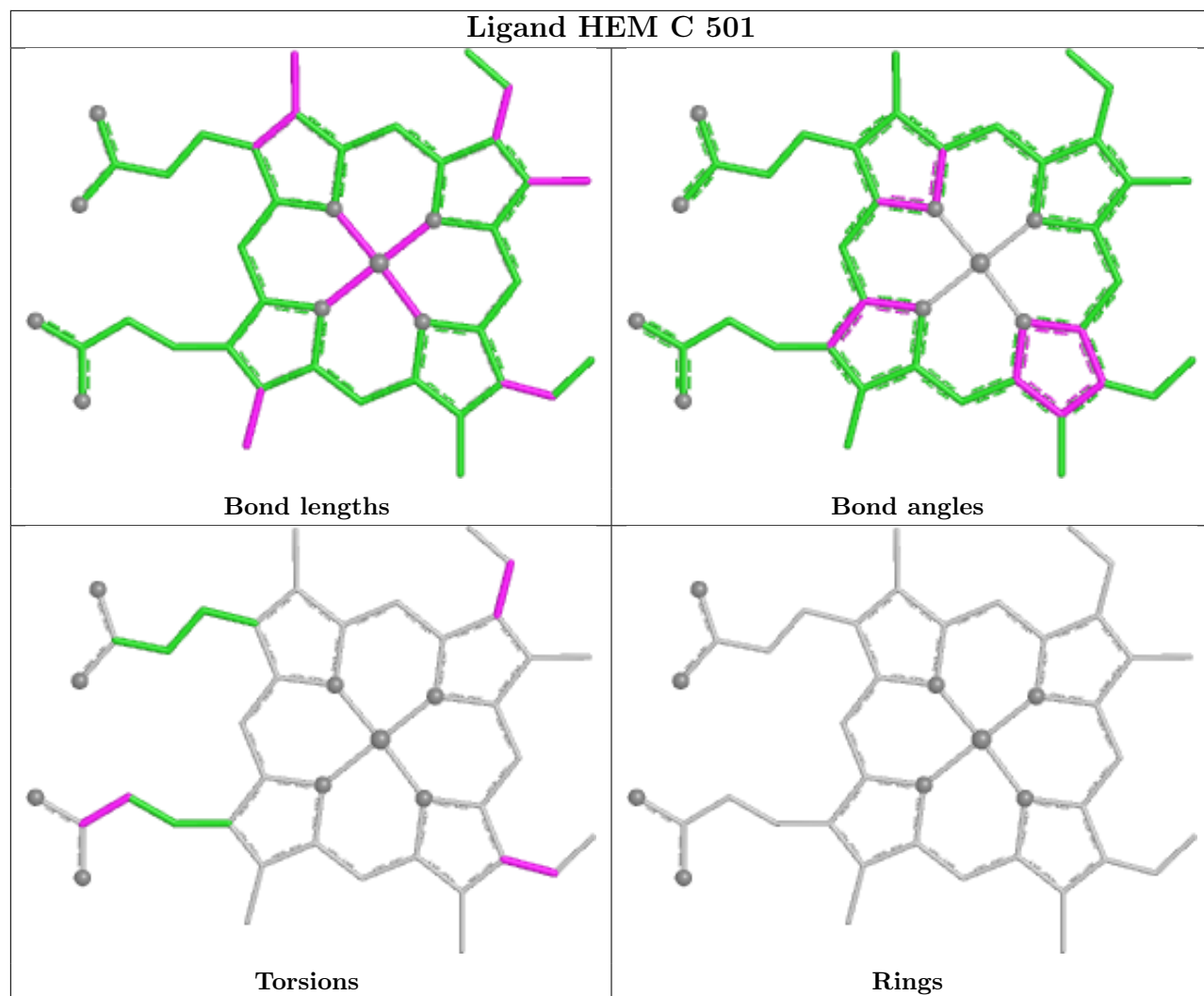
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

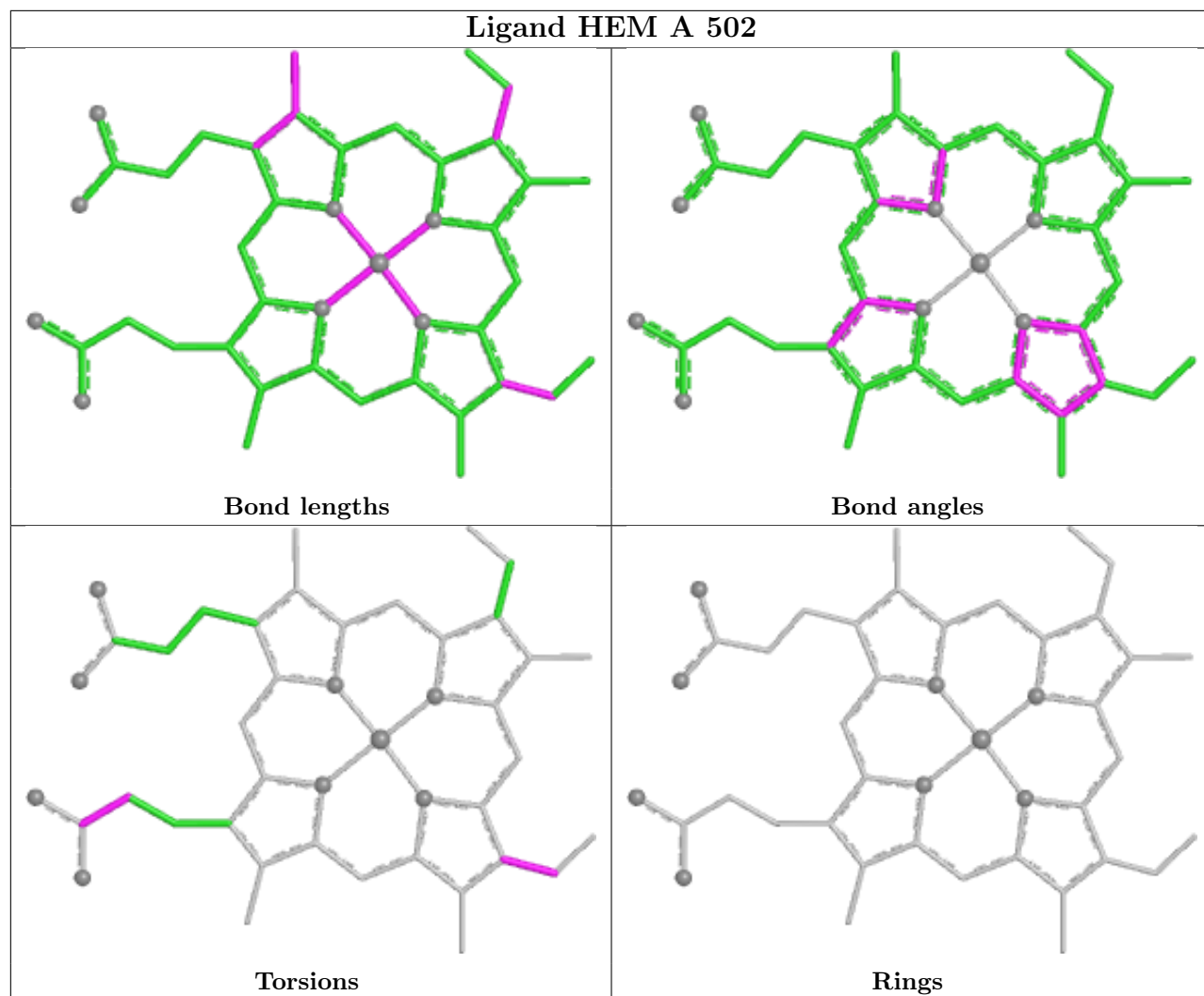












5.7 Other polymers [i](#)

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	464/476 (97%)	-1.42	0 100 100	32, 57, 74, 86	0
1	B	465/476 (97%)	-1.40	0 100 100	25, 59, 75, 95	0
1	C	464/476 (97%)	-1.34	0 100 100	40, 69, 92, 102	0
1	D	465/476 (97%)	-1.40	0 100 100	39, 62, 81, 93	0
1	E	465/476 (97%)	-1.35	0 100 100	41, 70, 96, 106	0
1	F	465/476 (97%)	-1.39	0 100 100	39, 62, 81, 92	0
All	All	2788/2856 (97%)	-1.38	0 100 100	25, 63, 86, 106	0

There are no RSRZ outliers to report.

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	SNE	B	502	10/10	0.96	0.12	63,64,65,65	0

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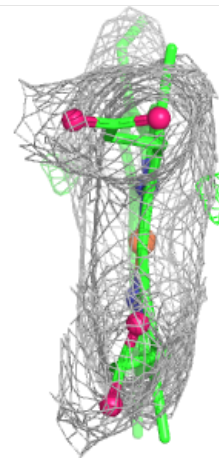
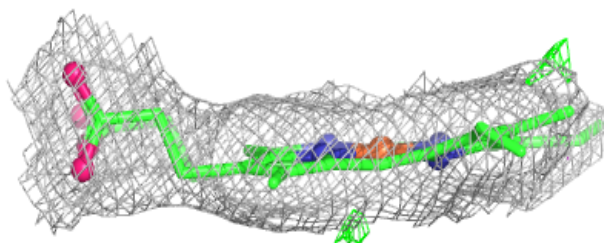
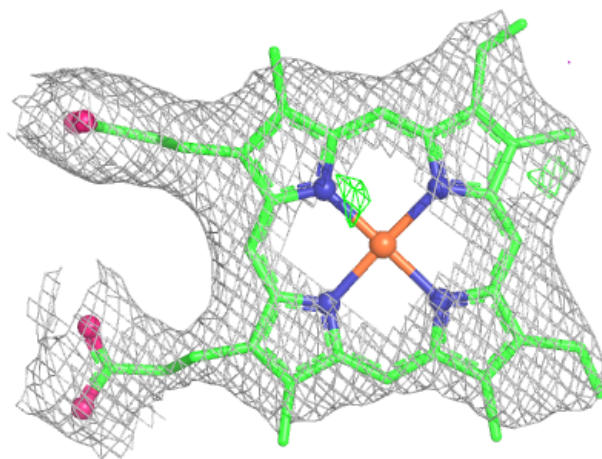
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SNE	D	502	10/10	0.97	0.09	54,58,58,59	0
3	SNE	E	502	10/10	0.97	0.11	83,83,84,84	0
3	SNE	C	502	10/10	0.98	0.10	89,90,90,90	0
3	SNE	A	501	10/10	0.98	0.10	63,64,64,65	0
2	HEM	F	501	43/43	0.99	0.05	55,60,62,62	0
2	HEM	C	501	43/43	0.99	0.04	51,59,61,61	0
2	HEM	E	501	43/43	0.99	0.04	49,55,62,65	0
3	SNE	F	502	10/10	0.99	0.09	94,95,96,96	0
2	HEM	D	501	43/43	1.00	0.04	32,44,47,48	0
2	HEM	A	502	43/43	1.00	0.03	42,46,48,49	0
2	HEM	B	501	43/43	1.00	0.04	36,43,47,49	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.

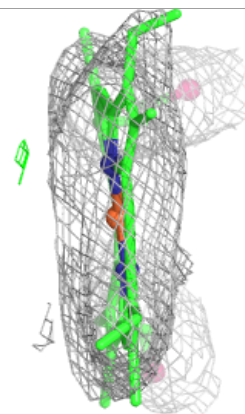
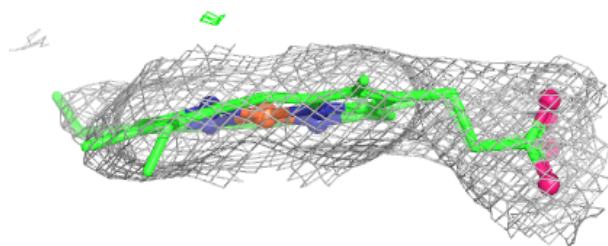
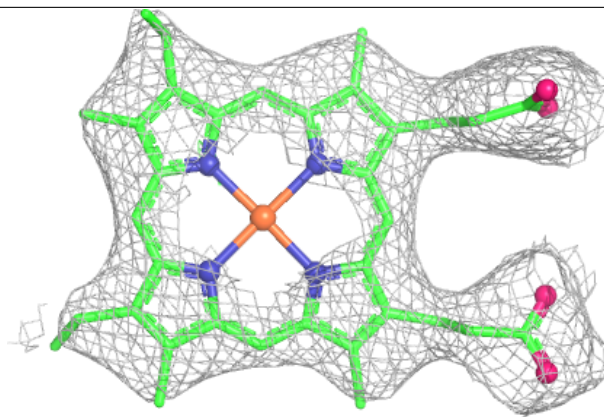
Electron density around HEM F 501:

2mF_o-DF_c (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
 and green (positive)



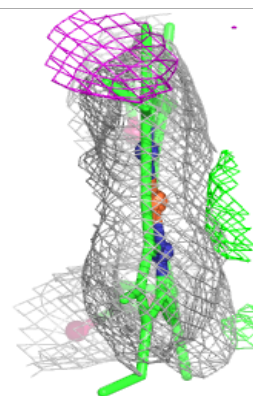
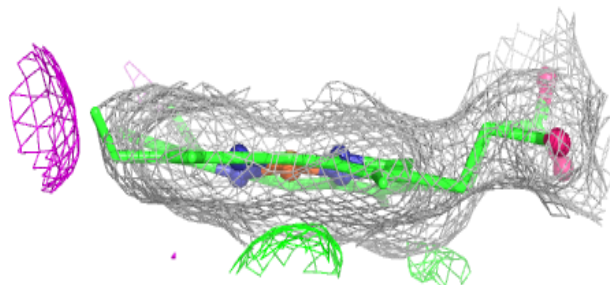
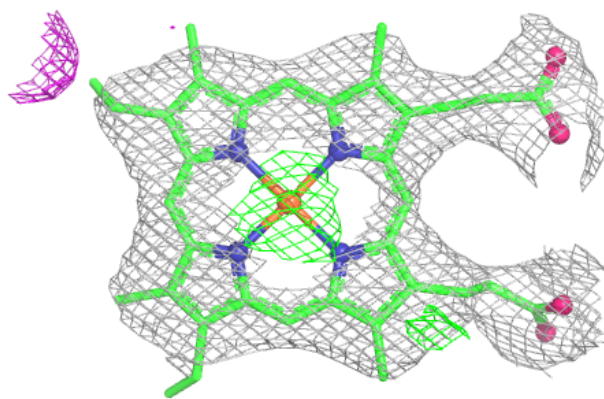
Electron density around HEM C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



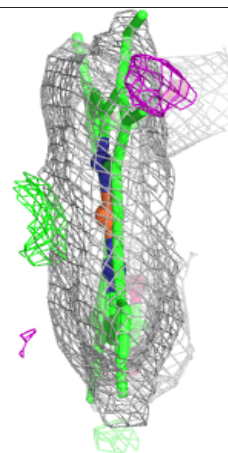
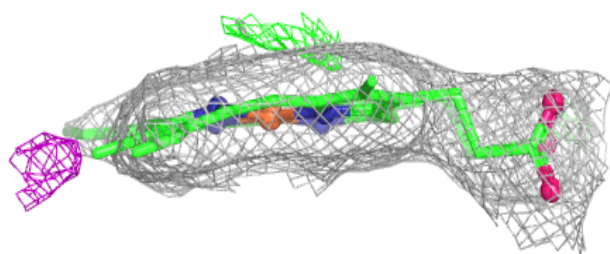
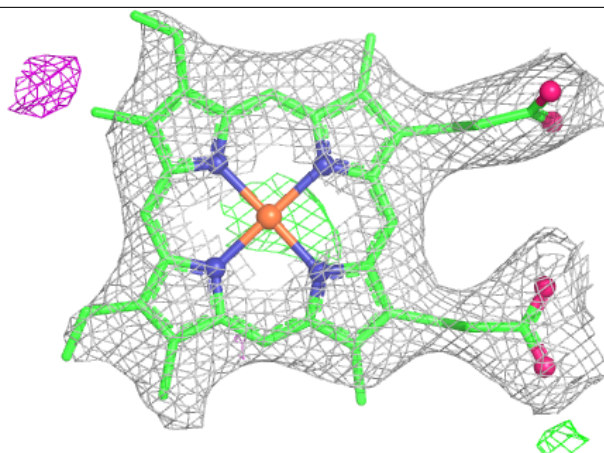
Electron density around HEM E 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



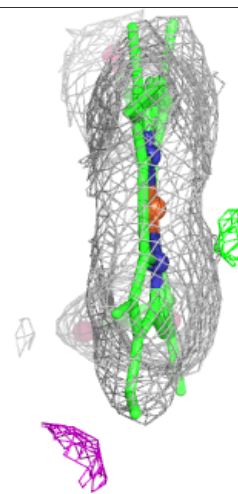
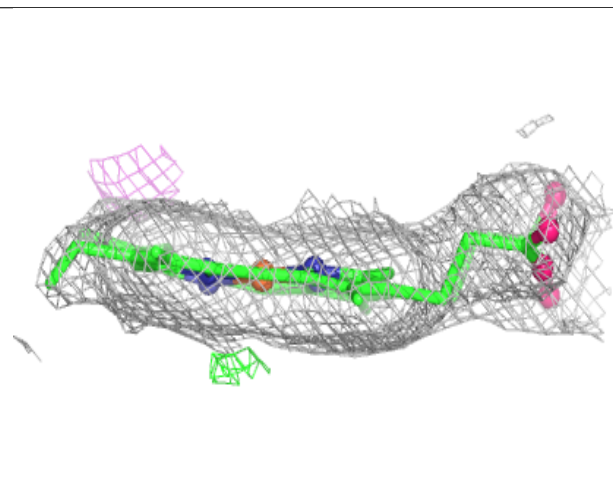
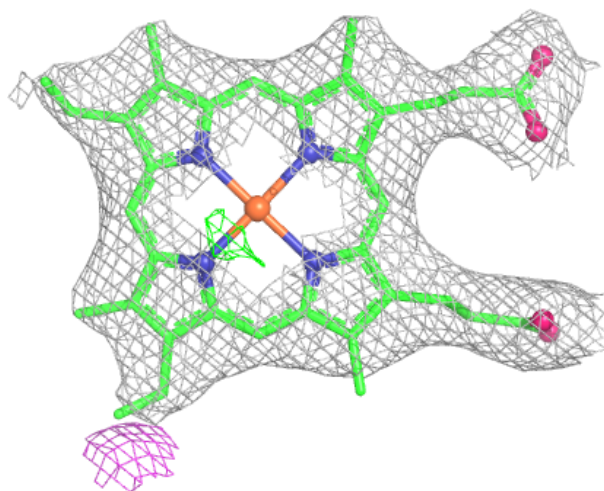
Electron density around HEM D 501:

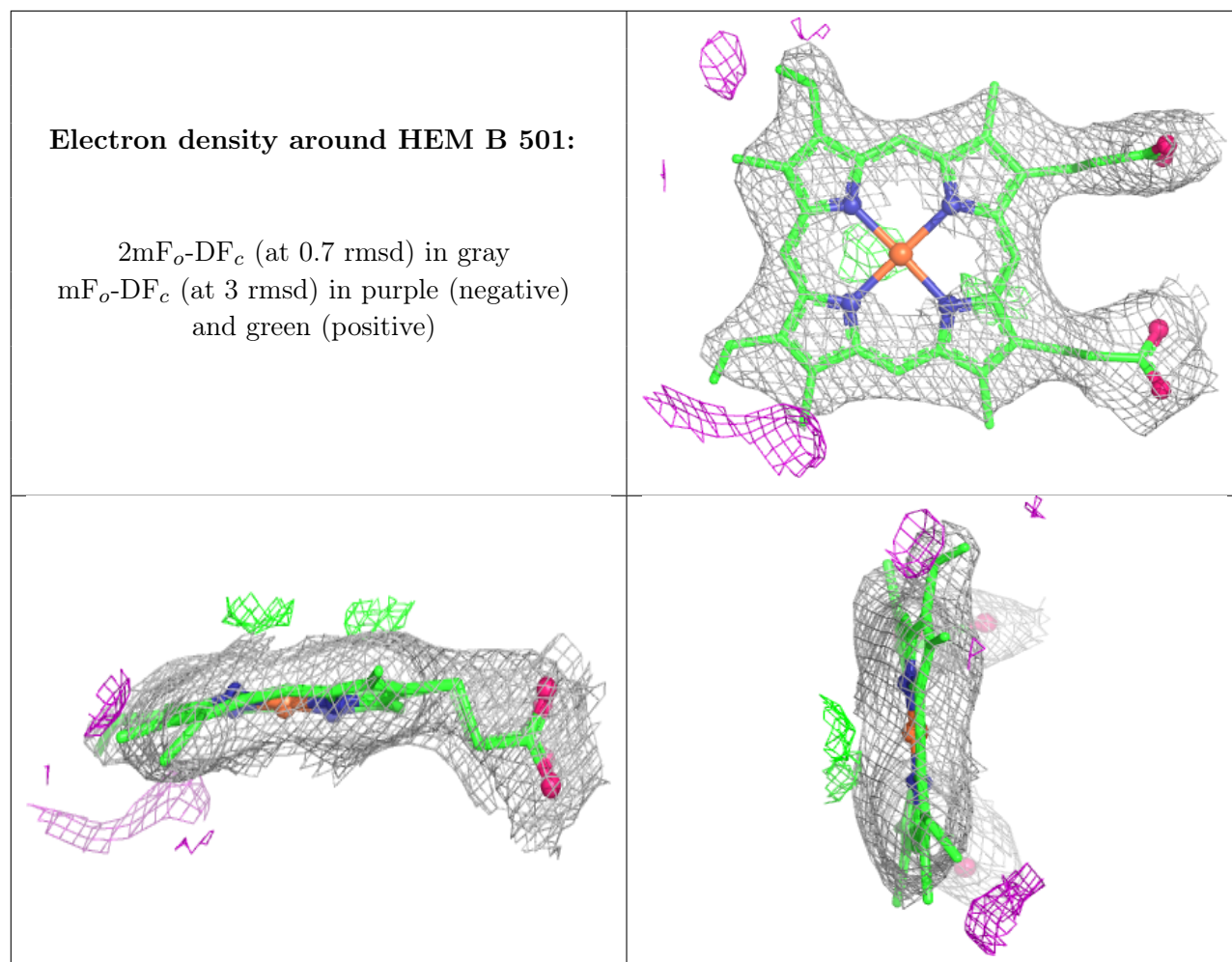
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.