Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 02:20 PM EDT

PDB ID	:	3VRA / pdb_00003vra
Title	:	Mitochondrial rhodoquinol-fumarate reductase from the parasitic nematode Ascaris suum with the specific inhibitor Atpenin A5
Authors	:	Shimizu, H.; Shiba, T.; Inaoka, D.K.; Osanai, A.; Kita, K.; Sakamoto, K.; Harada, S.
Deposited on	:	2012-04-07
Resolution	:	3.44 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 (i) 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 (i)) were used in the production of this report:

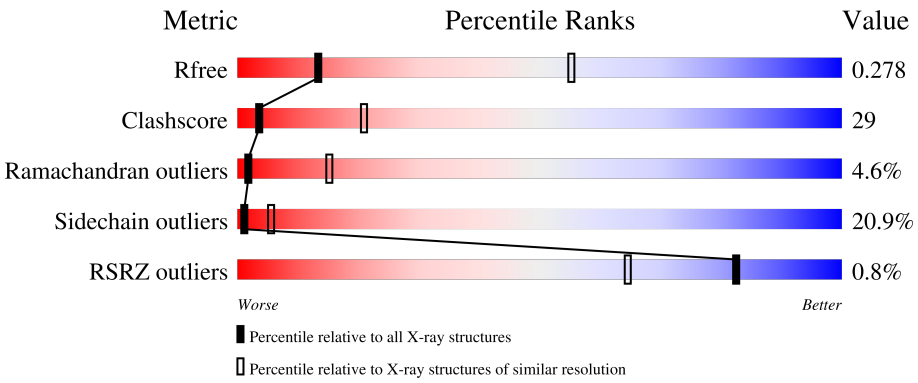
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.44 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	1736 (3.50-3.38)
Clashscore	190562	1808 (3.50-3.38)
Ramachandran outliers	187476	1776 (3.50-3.38)
Sidechain outliers	187428	1777 (3.50-3.38)
RSRZ outliers	180081	1736 (3.50-3.38)

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 <=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	645	% 40% 43% 11% • 5%
1	E	645	% 38% 46% 10% • 5%
2	B	282	32% 43% 12% • 12%
2	F	282	% 39% 33% 15% • 12%

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Mol	Chain	Length	Quality of chain
3	C	188	%, 27%, 44%, 9%, •, 19%
3	G	188	%, 29%, 43%, 9%, •, 19%
4	D	156	44%, 31%, 6%, •, 17%
4	H	156	3%, 35%, 37%, 10%, •, 17%

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
11	AT5	C	202	-	-	X	-
11	AT5	G	202	-	-	X	-
5	MLI	A	701	-	-	X	-
5	MLI	E	701	-	X	X	-
8	SF4	B	302	-	-	X	-
9	F3S	F	303	-	-	X	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 18262 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 Flavoprotein subunit of complex II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	613	4758	2983	851	896	28	0	0	0
1	E	613	4758	2983	851	896	28	0	0	0

- Molecule 2 is a protein called Iron-sulfur subunit of succinate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	249	1973	1254	337	359	23	0	0	0
2	F	249	1973	1254	337	359	23	0	0	0

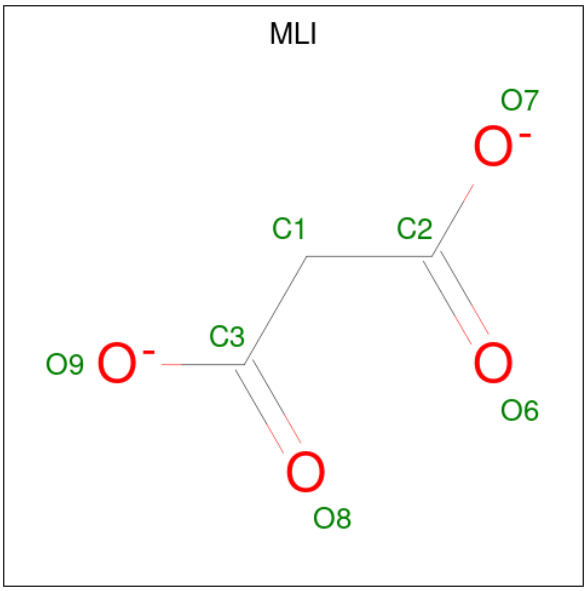
- Molecule 3 is a protein called Cytochrome b-large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	153	1217	813	204	194	6	0	0	0
3	G	153	1217	813	204	194	6	0	0	0

- Molecule 4 is a protein called Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial.

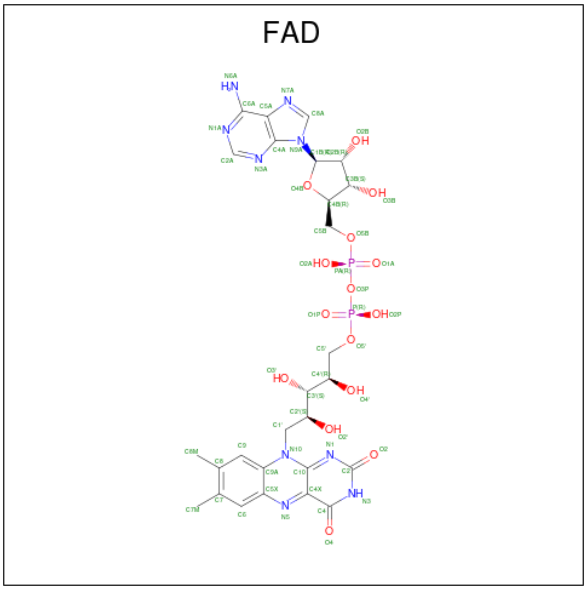
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	129	994	658	165	166	5	0	0	0
4	H	129	994	658	165	166	5	0	0	0

- Molecule 5 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



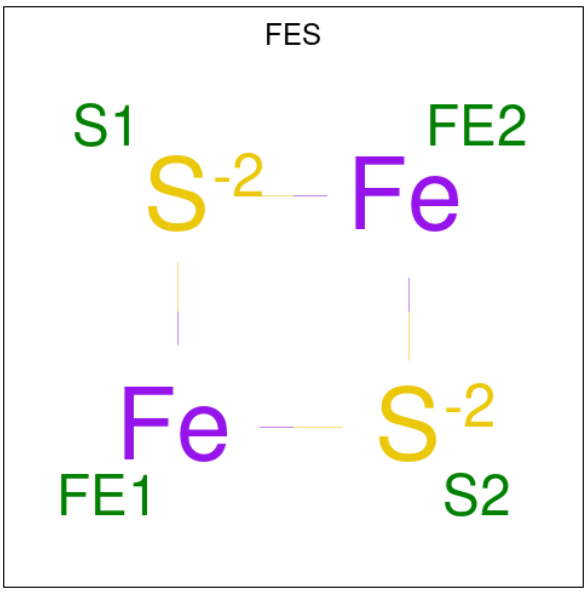
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
5	A	1	7	3	4		0	0
			Total	C	O			
5	E	1	7	3	4		0	0

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



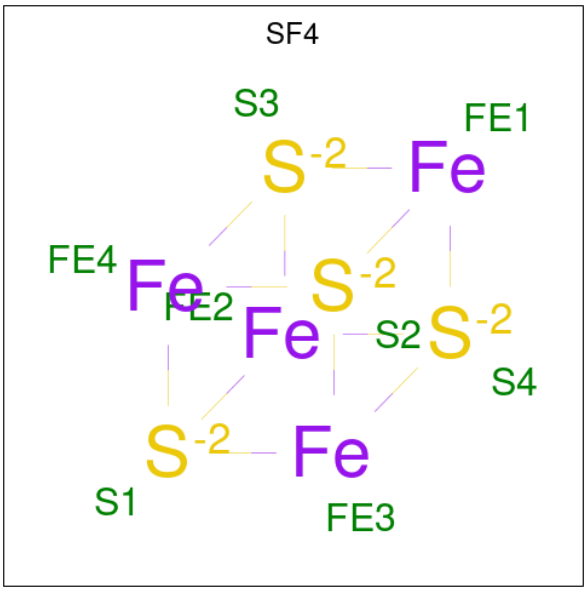
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
6	E	1	53	27	9	15	2	0	0

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
7	B	1	4	2	2	0	0
7	F	1	4	2	2	0	0

- Molecule 8 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
8	B	1	8	4	4	0	0

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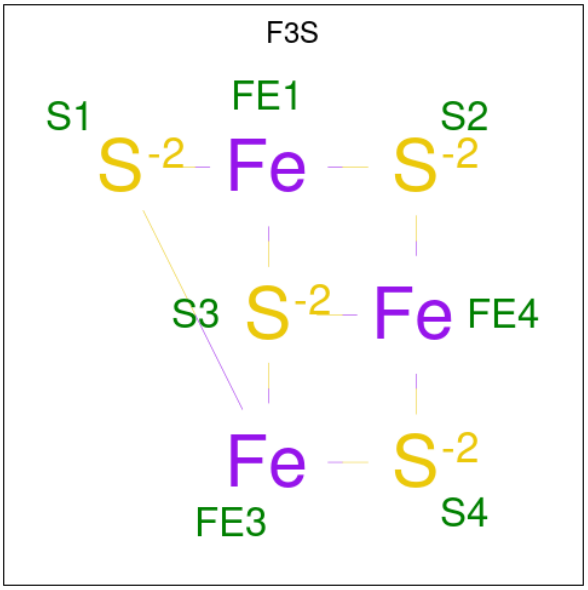
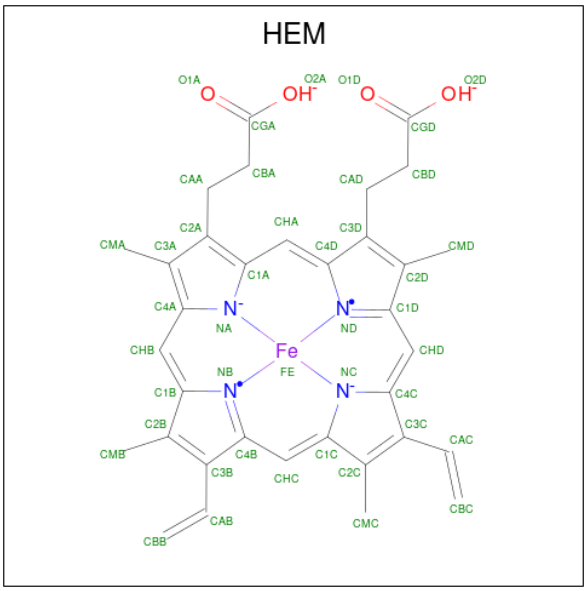
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
8	F	1	8	4	4	0	0

- Molecule 9 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



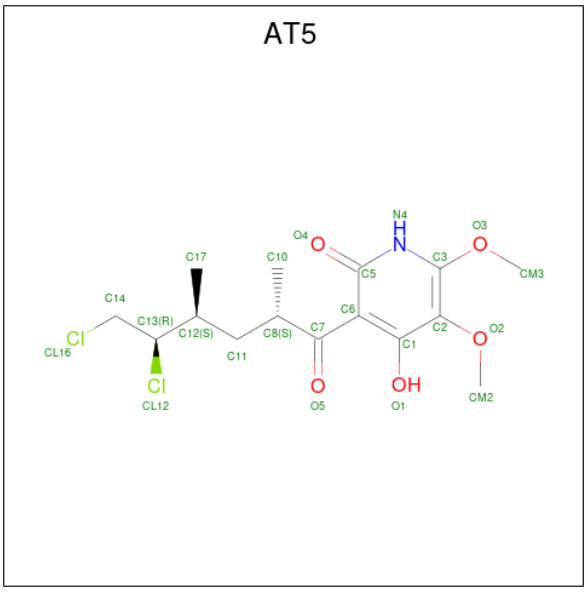
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
9	B	1	7	3	4	0	0
9	F	1	7	3	4	0	0

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 11 is 3-[(2S,4S,5R)-5,6-DICHLORO-2,4-DIMETHYL-1-OXOHEXYL]-4-HYDROXY-5,6-DIMETHOXY-2(1H)-PYRIDINONE (CCD ID: AT5) (formula: $C_{15}H_{21}Cl_2NO_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
11	C	1	23	15	2	1	5	0	0

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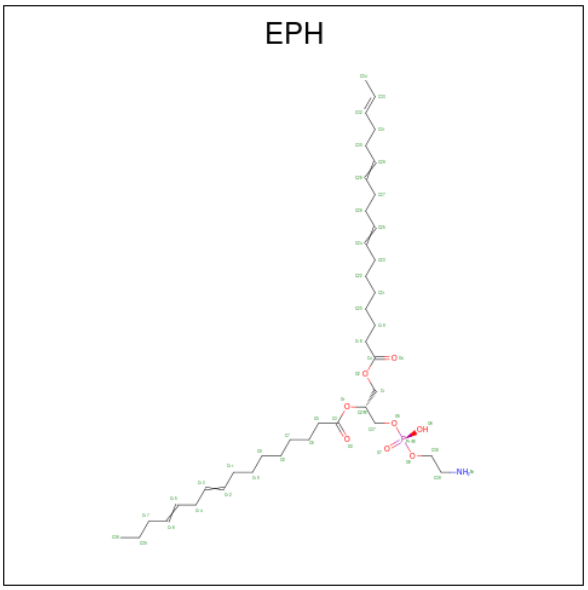
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
11	G	1	23	15	2	1	5	0	0

- Molecule 12 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (CCD ID: EPH) (formula: $C_{39}H_{68}NO_8P$).



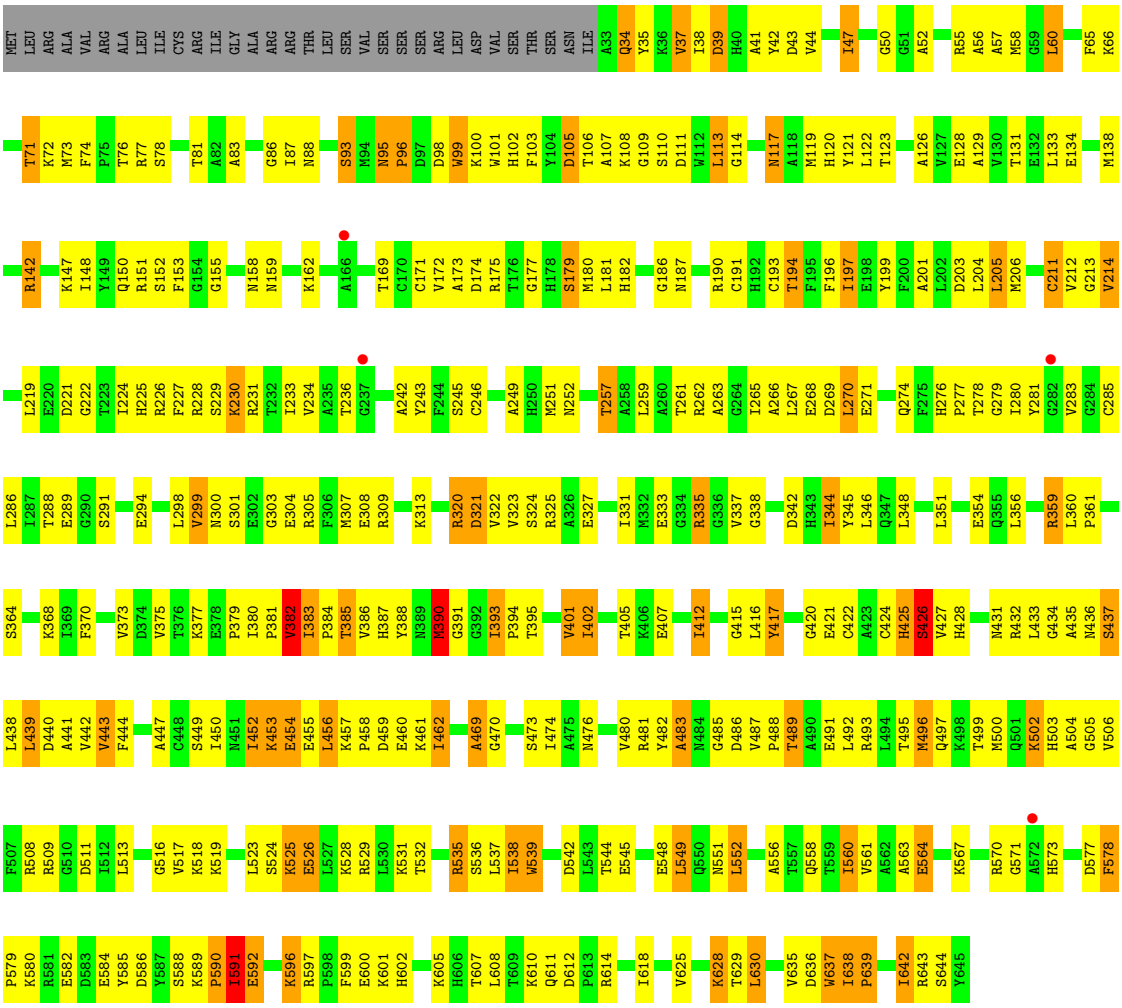
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
12	D	1	44	34	1	8	1	0	0
			Total	C	N	O	P		
12	H	1	44	34	1	8	1	0	0

3 Residue-property plots (i)

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

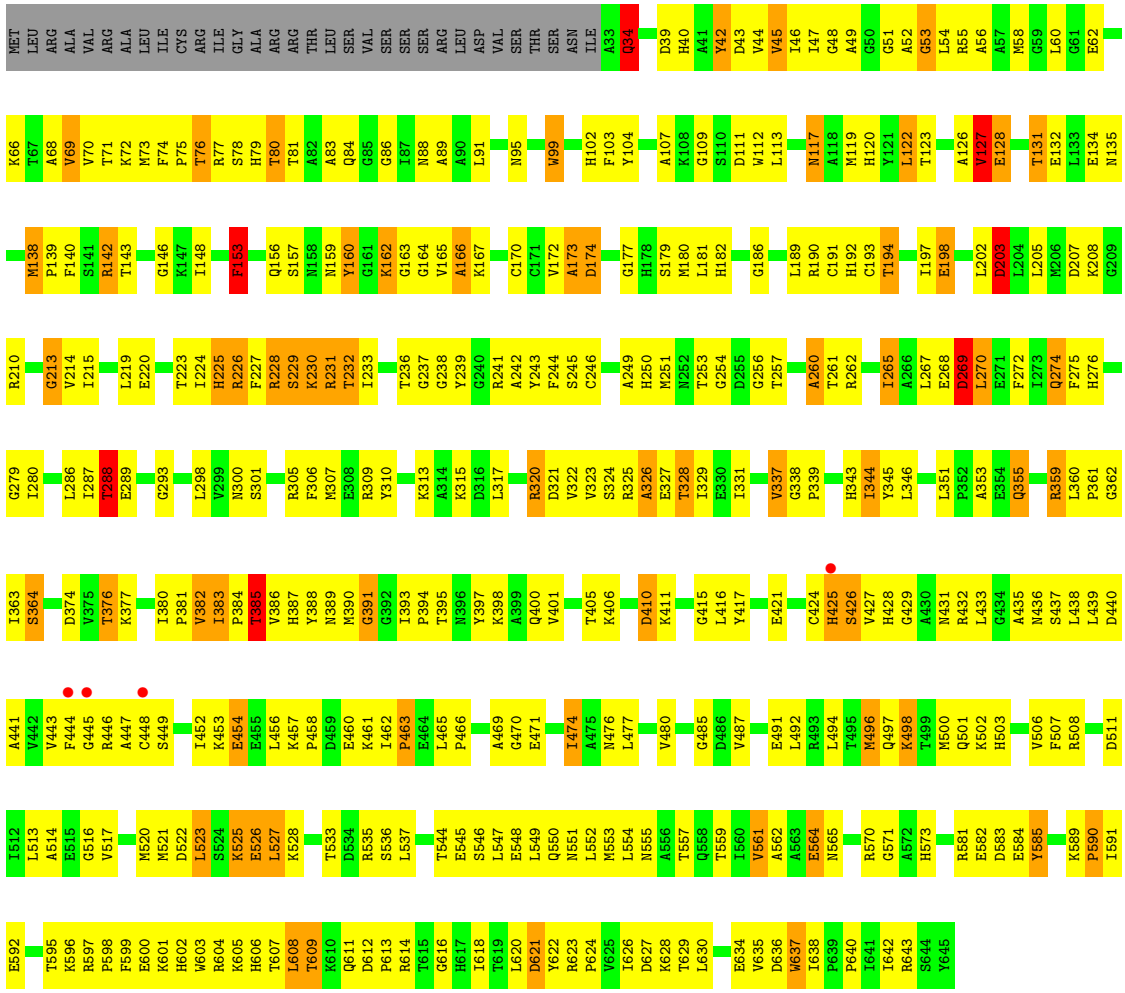
• Molecule 1: Flavoprotein subunit of complex II

Chain A:



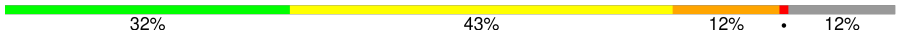
• Molecule 1: Flavoprotein subunit of complex II

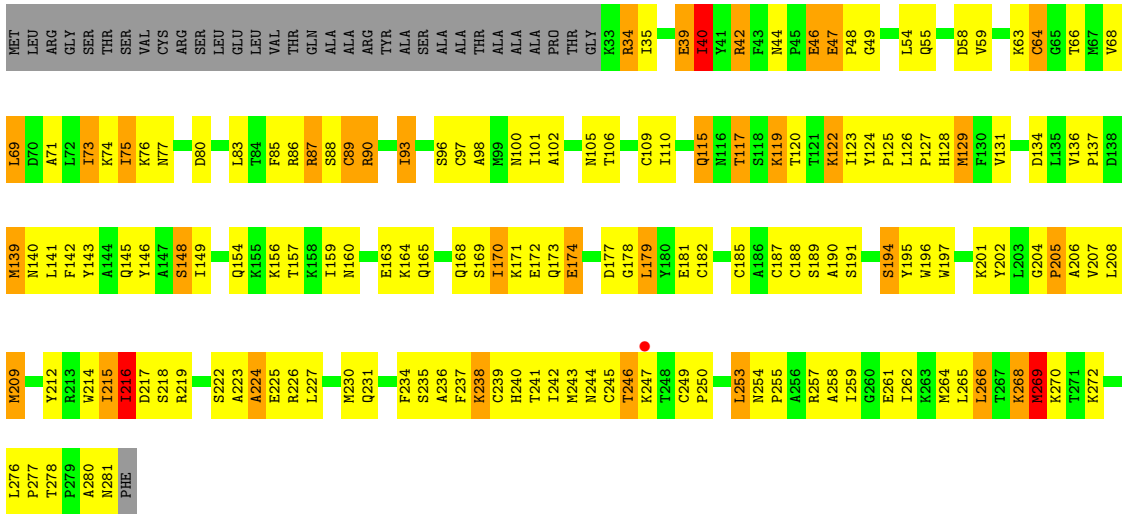
Chain E:



• Molecule 2: Iron-sulfur subunit of succinate dehydrogenase

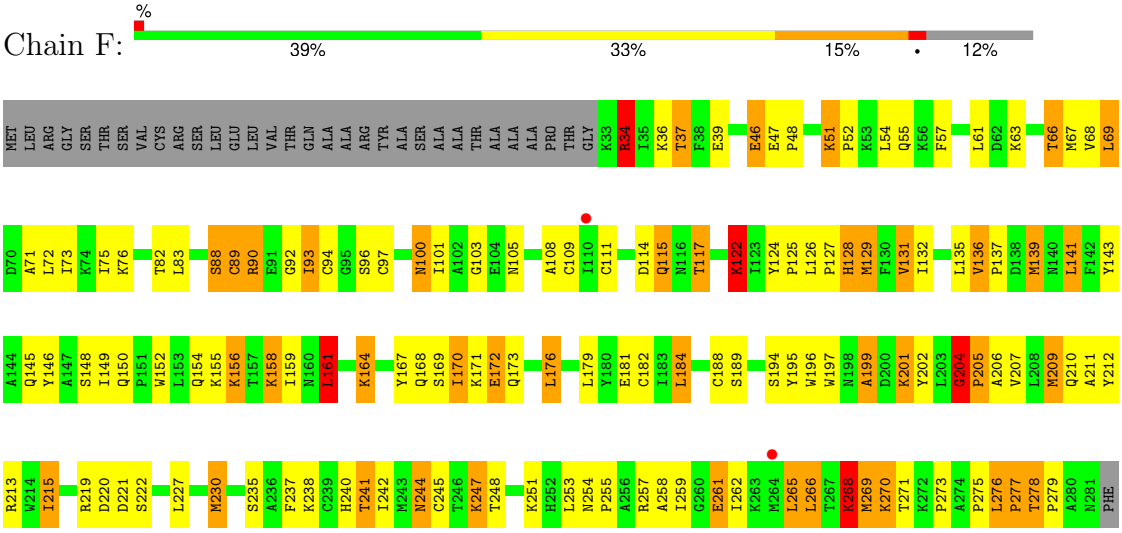
Chain B:





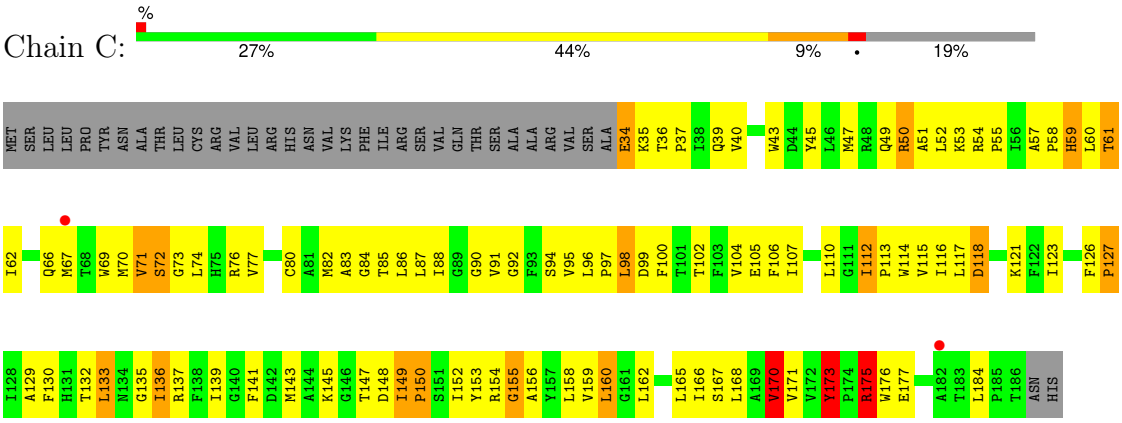
• Molecule 2: Iron-sulfur subunit of succinate dehydrogenase

Chain F:



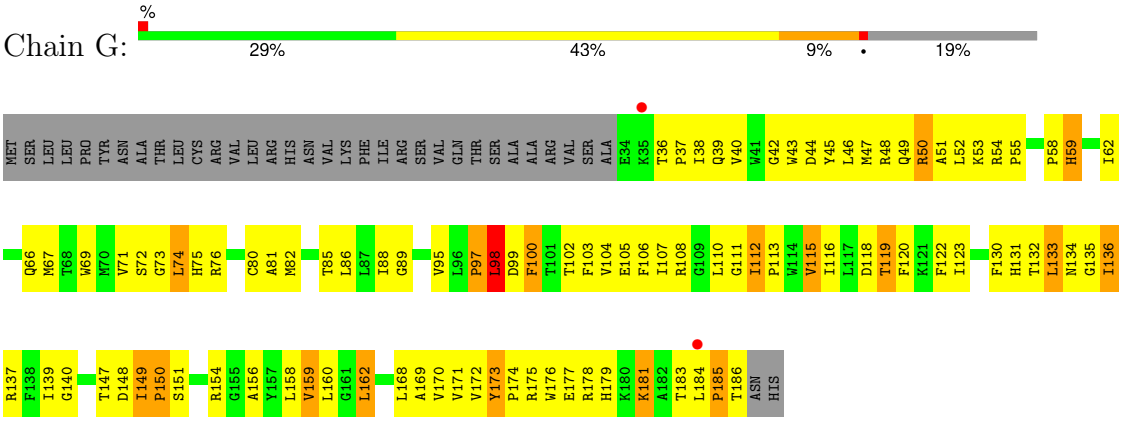
• Molecule 3: Cytochrome b-large subunit

Chain C:



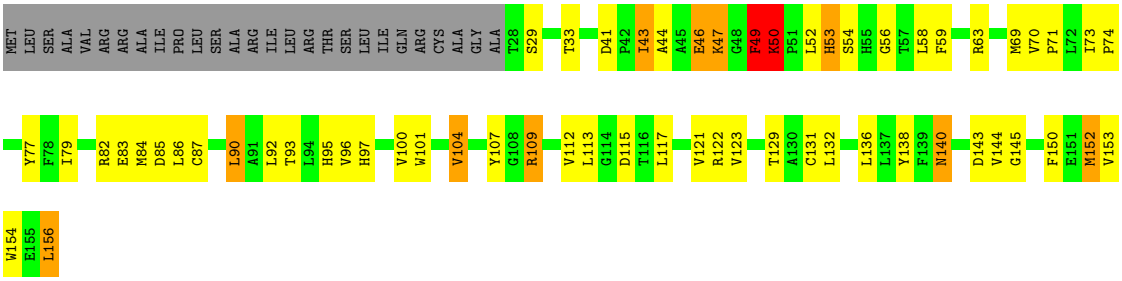
• Molecule 3: Cytochrome b-large subunit

Chain G:



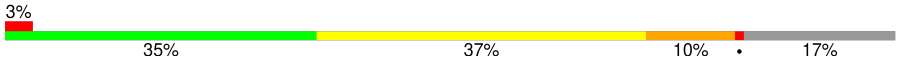
• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial

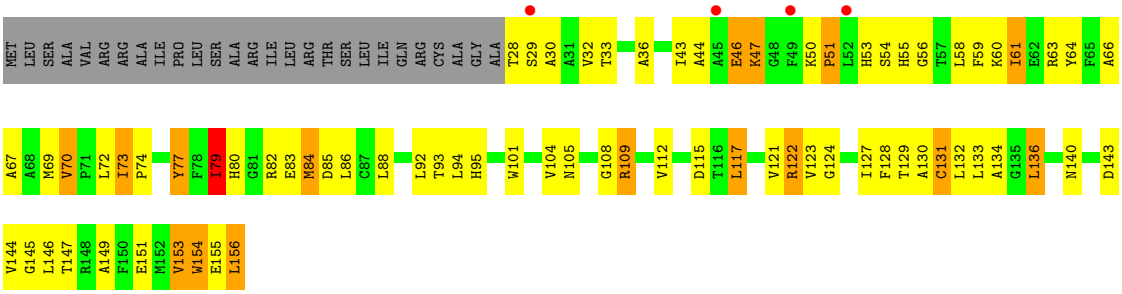
Chain D:



• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	122.82Å 132.25Å 220.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 3.44 49.72 – 3.44	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.72-3.44) 89.4 (49.72-3.44)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.205 , 0.281 0.203 , 0.278	Depositor DCC
R_{free} test set	2217 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	103.9	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18262	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MLI, HEM, SF4, AT5, F3S, FAD, EPH, FES

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	0.82	1/4859 (0.0%)	1.12	19/6564 (0.3%)
1	E	0.84	0/4859	1.20	33/6564 (0.5%)
2	B	0.91	0/2016	1.20	9/2723 (0.3%)
2	F	0.97	2/2016 (0.1%)	1.30	17/2723 (0.6%)
3	C	0.89	0/1255	1.19	12/1709 (0.7%)
3	G	0.95	2/1255 (0.2%)	1.23	7/1709 (0.4%)
4	D	0.89	1/1026 (0.1%)	1.18	3/1402 (0.2%)
4	H	0.93	2/1026 (0.2%)	1.16	2/1402 (0.1%)
All	All	0.88	8/18312 (0.0%)	1.19	102/24796 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	136	ILE	CA-CB	6.14	1.61	1.54
4	H	79	ILE	CA-CB	5.84	1.60	1.54
3	G	115	VAL	CA-CB	5.69	1.61	1.54
4	H	32	VAL	CA-CB	5.65	1.60	1.54
2	F	170	ILE	CA-CB	5.60	1.61	1.54
1	A	412	ILE	CA-CB	5.31	1.59	1.54
4	D	49	PHE	N-CA	5.21	1.52	1.46
2	F	82	THR	CA-CB	5.21	1.61	1.53

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	589	LYS	CA-C-N	9.58	131.81	119.84
1	E	589	LYS	C-N-CA	9.58	131.81	119.84
2	F	270	LYS	N-CA-C	9.12	123.01	109.24
2	F	204	GLY	CA-C-N	9.01	131.10	119.84
2	F	204	GLY	C-N-CA	9.01	131.10	119.84
2	F	136	VAL	N-CA-C	8.83	115.59	107.56
1	E	143	THR	CA-C-N	-8.77	110.57	120.04
1	E	143	THR	C-N-CA	-8.77	110.57	120.04
2	B	204	GLY	CA-C-N	8.57	130.56	119.84
2	B	204	GLY	C-N-CA	8.57	130.56	119.84
2	F	122	LYS	N-CA-C	8.39	123.10	109.59
4	H	32	VAL	N-CA-C	8.14	120.63	109.80
2	F	269	MET	N-CA-C	7.71	120.28	110.33
1	A	578	PHE	CA-C-N	7.59	127.30	119.56
1	A	578	PHE	C-N-CA	7.59	127.30	119.56
1	A	373	VAL	N-CA-C	7.00	117.94	107.51
3	G	173	TYR	CA-C-N	-6.90	111.21	119.84
3	G	173	TYR	C-N-CA	-6.90	111.21	119.84
4	D	53	HIS	N-CA-C	6.88	118.89	109.11
1	E	383	ILE	CA-C-N	-6.88	112.85	120.14
1	E	383	ILE	C-N-CA	-6.88	112.85	120.14
1	E	385	THR	N-CA-C	6.84	120.31	109.50
1	E	425	HIS	N-CA-C	-6.71	104.82	112.87
1	A	382	VAL	N-CA-C	6.69	117.75	108.12
4	H	79	ILE	CB-CA-C	6.66	118.88	111.08
2	B	216	ILE	CB-CA-C	-6.62	104.58	112.19
1	A	186	GLY	N-CA-C	-6.62	104.83	112.50
3	G	106	PHE	N-CA-C	-6.59	104.47	113.30
2	B	178	GLY	N-CA-C	-6.58	106.36	114.92
1	E	153	PHE	N-CA-C	6.56	117.13	108.07
3	C	173	TYR	CA-C-N	-6.55	112.97	120.89
3	C	173	TYR	C-N-CA	-6.55	112.97	120.89
2	B	40	ILE	N-CA-C	6.41	117.25	107.77
2	F	278	THR	CA-C-N	6.26	127.67	119.84
2	F	278	THR	C-N-CA	6.26	127.67	119.84
1	E	213	GLY	N-CA-C	6.15	118.25	110.38
1	E	174	ASP	N-CA-C	-6.13	107.03	114.75
1	E	166	ALA	N-CA-C	6.09	119.53	110.52
2	F	141	LEU	N-CA-C	-6.03	104.40	110.97
2	F	51	LYS	CA-C-N	5.98	127.32	119.84
2	F	51	LYS	C-N-CA	5.98	127.32	119.84
2	B	66	THR	N-CA-C	5.90	117.79	111.36
1	E	338	GLY	CA-C-N	5.90	127.21	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	338	GLY	C-N-CA	5.90	127.21	119.84
1	E	42	TYR	N-CA-C	5.88	118.70	108.76
3	C	36	THR	CA-C-N	5.88	127.19	119.84
3	C	36	THR	C-N-CA	5.88	127.19	119.84
1	E	465	LEU	CA-C-N	5.86	125.88	119.90
1	E	465	LEU	C-N-CA	5.86	125.88	119.90
1	A	393	ILE	CA-C-N	5.85	127.15	119.84
1	A	393	ILE	C-N-CA	5.85	127.15	119.84
1	E	229	SER	N-CA-C	5.83	117.89	108.32
1	E	138	MET	CA-C-N	5.82	127.12	119.84
1	E	138	MET	C-N-CA	5.82	127.12	119.84
2	F	220	ASP	N-CA-C	5.70	117.98	109.25
1	A	171	CYS	N-CA-C	5.69	117.66	108.32
1	E	382	VAL	N-CA-C	5.64	116.24	107.28
3	C	175	ARG	N-CA-C	-5.62	106.42	113.28
1	E	315	LYS	N-CA-C	5.61	116.83	108.31
2	B	270	LYS	N-CA-C	5.59	118.81	110.14
1	E	69	VAL	N-CA-C	5.58	114.77	106.85
2	B	269	MET	N-CA-C	5.57	118.07	110.55
1	E	142	ARG	N-CA-C	5.55	118.28	109.50
3	C	57	ALA	CA-C-N	5.53	126.75	119.84
3	C	57	ALA	C-N-CA	5.53	126.75	119.84
3	C	170	VAL	N-CA-C	-5.53	108.11	113.53
3	C	40	VAL	CB-CA-C	-5.51	104.65	111.70
3	G	100	PHE	N-CA-C	5.47	116.92	111.07
3	G	176	TRP	N-CA-C	-5.47	105.23	112.94
1	A	197	ILE	N-CA-C	5.44	116.72	109.37
1	A	402	ILE	N-CA-C	5.43	115.95	108.12
1	E	203	ASP	N-CA-C	5.41	117.07	108.79
1	E	34	GLN	N-CA-C	5.38	117.28	108.52
3	G	154	ARG	N-CA-C	-5.36	104.48	111.02
1	E	454	GLU	N-CA-C	5.35	117.11	111.28
1	A	390	MET	N-CA-C	-5.34	104.50	111.02
1	E	225	HIS	N-CA-C	5.34	117.10	108.34
1	A	437	SER	N-CA-C	5.33	116.89	111.14
2	F	47	GLU	CA-C-N	5.33	126.50	119.84
2	F	47	GLU	C-N-CA	5.33	126.50	119.84
4	D	115	ASP	N-CA-C	5.32	116.76	111.07
1	E	457	LYS	CA-C-N	5.31	126.48	119.84
1	E	457	LYS	C-N-CA	5.31	126.48	119.84
1	A	95	ASN	CA-C-N	5.30	126.47	119.84
1	A	95	ASN	C-N-CA	5.30	126.47	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	639	PRO	CA-C-N	5.29	126.45	119.84
1	A	639	PRO	C-N-CA	5.29	126.45	119.84
3	G	159	VAL	N-CA-C	5.27	116.00	110.62
1	E	86	GLY	N-CA-C	5.25	117.51	110.43
3	C	184	LEU	CA-C-N	5.23	124.68	119.24
3	C	184	LEU	C-N-CA	5.23	124.68	119.24
1	A	364	SER	N-CA-C	-5.22	105.70	111.71
1	E	565	ASN	N-CA-C	5.19	118.77	112.23
3	C	40	VAL	N-CA-C	-5.18	104.84	110.23
2	B	87	ARG	N-CA-C	5.13	117.53	108.75
2	F	34	ARG	N-CA-C	5.13	117.07	107.99
1	A	245	SER	N-CA-C	5.12	116.76	108.41
1	E	194	THR	CB-CA-C	5.10	118.74	110.22
4	D	50	LYS	N-CA-C	5.10	121.08	109.81
1	A	637	TRP	CA-CB-CG	5.08	123.25	113.60
2	F	244	ASN	N-CA-C	5.07	117.19	111.11
2	F	164	LYS	N-CA-C	5.01	116.14	108.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	425	HIS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4758	0	4692	275	0
1	E	4758	0	4692	299	0
2	B	1973	0	1994	145	0
2	F	1973	0	1994	137	0
3	C	1217	0	1265	96	0
3	G	1217	0	1265	74	0
4	D	994	0	977	50	0
4	H	994	0	977	62	0
5	A	7	0	2	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	7	0	2	4	0
6	A	53	0	30	12	0
6	E	53	0	31	18	0
7	B	4	0	0	0	0
7	F	4	0	0	1	0
8	B	8	0	0	5	0
8	F	8	0	0	0	0
9	B	7	0	0	0	0
9	F	7	0	0	2	0
10	C	43	0	30	14	0
10	G	43	0	30	15	0
11	C	23	0	20	12	0
11	G	23	0	21	11	0
12	D	44	0	53	4	0
12	H	44	0	53	2	0
All	All	18262	0	18128	1070	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 29.

All (1070) 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:E:79:HIS:NE2	6:E:702:FAD:HM81	1.10	1.36
1:E:79:HIS:NE2	6:E:702:FAD:C8M	1.89	1.35
3:C:114:TRP:HB2	3:C:175:ARG:HH11	1.09	1.14
2:F:115:GLN:HE21	2:F:115:GLN:HA	1.14	1.08
3:C:107:ILE:HD11	4:D:156:LEU:HD22	1.35	1.07
1:A:83:ALA:HB3	1:A:177:GLY:HA3	1.33	1.07
3:G:149:ILE:HD13	3:G:149:ILE:H	1.14	1.06
10:G:201:HEM:HMB1	10:G:201:HEM:HBB2	1.39	1.04
4:D:109:ARG:HG2	4:D:109:ARG:HH21	1.15	1.04
1:A:44:VAL:HG11	1:A:60:LEU:HD22	1.37	1.03
2:F:131:VAL:HG23	3:G:55:PRO:HG2	1.39	1.02
1:A:321:ASP:HB3	1:A:431:ASN:ND2	1.75	1.01
1:A:190:ARG:HA	4:D:43:ILE:HD11	1.42	1.00
3:C:123:ILE:O	3:C:127:PRO:HD2	1.60	0.99
2:F:268:LYS:CG	2:F:269:MET:H	1.75	0.98
1:E:79:HIS:CD2	6:E:702:FAD:C8M	2.46	0.98
2:F:240:HIS:HB2	11:G:202:AT5:HM31	1.45	0.98
3:C:149:ILE:HD13	3:C:149:ILE:H	1.27	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:570:ARG:NH1	1:E:581:ARG:HD2	1.81	0.95
2:F:240:HIS:CB	11:G:202:AT5:HM31	1.97	0.93
2:F:105:ASN:HD21	2:F:127:PRO:HD2	1.33	0.92
1:A:503:HIS:HD2	1:A:516:GLY:HA2	1.32	0.92
1:E:79:HIS:CD2	6:E:702:FAD:HM83	2.03	0.92
3:G:133:LEU:O	3:G:136:ILE:HG13	1.68	0.92
1:E:561:VAL:HG21	1:E:618:ILE:HG21	1.50	0.91
2:F:57:PHE:CD2	2:F:75:ILE:HD12	2.05	0.91
10:C:201:HEM:HMB1	10:C:201:HEM:HBB2	1.52	0.90
4:H:50:LYS:N	4:H:51:PRO:HD2	1.86	0.90
2:F:89:CYS:HG	7:F:301:FES:FE2	0.67	0.90
1:A:213:GLY:HA3	1:A:227:PHE:O	1.71	0.90
1:E:583:ASP:O	1:E:602:HIS:HB2	1.71	0.89
1:A:274:GLN:HB2	1:A:390:MET:HE1	1.55	0.89
1:E:582:GLU:HB2	1:E:603:TRP:HD1	1.38	0.88
11:G:202:AT5:HM23	11:G:202:AT5:HM32	1.54	0.87
1:E:43:ASP:OD2	1:E:230:LYS:HE2	1.75	0.87
1:E:583:ASP:O	1:E:602:HIS:CB	2.23	0.87
2:F:115:GLN:HA	2:F:115:GLN:NE2	1.82	0.87
2:B:240:HIS:HB2	11:C:202:AT5:HM31	1.57	0.87
2:F:268:LYS:HG3	2:F:269:MET:H	1.37	0.87
3:G:112:ILE:HB	3:G:113:PRO:CD	2.05	0.86
1:E:611:GLN:HG3	1:E:618:ILE:HG13	1.57	0.86
1:A:321:ASP:HB3	1:A:431:ASN:HD22	1.41	0.86
2:B:71:ALA:O	2:B:75:ILE:HG12	1.76	0.85
10:G:201:HEM:NC	4:H:95:HIS:CD2	2.44	0.84
1:A:503:HIS:HD2	1:A:516:GLY:CA	1.89	0.84
2:F:34:ARG:HB2	2:F:117:THR:HG21	1.59	0.84
10:G:201:HEM:HBD1	10:G:201:HEM:HHA	1.57	0.84
1:E:527:LEU:HD11	1:E:553:MET:HG3	1.58	0.84
1:E:388:TYR:CE1	1:E:421:GLU:HG3	2.13	0.84
1:E:424:CYS:C	1:E:426:SER:H	1.86	0.83
4:H:70:VAL:O	4:H:74:PRO:HD2	1.77	0.83
3:G:149:ILE:H	3:G:149:ILE:CD1	1.88	0.83
1:A:488:PRO:HG2	1:A:491:GLU:HB2	1.61	0.82
1:E:135:ASN:ND2	2:F:161:LEU:O	2.11	0.82
1:E:428:HIS:HB3	1:E:432:ARG:HA	1.60	0.82
4:H:109:ARG:HG2	4:H:109:ARG:HH21	1.45	0.82
3:C:149:ILE:H	3:C:149:ILE:CD1	1.92	0.81
3:G:112:ILE:HB	3:G:113:PRO:HD3	1.60	0.81
1:A:222:GLY:HA3	1:A:537:LEU:HB3	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:82:MET:HE3	10:G:201:HEM:HAC	1.61	0.80
2:F:150:GLN:HG2	2:F:152:TRP:CH2	2.16	0.80
1:A:205:LEU:HB3	1:A:212:VAL:HG23	1.61	0.80
2:B:179:LEU:HD12	2:B:209:MET:HE2	1.63	0.80
1:E:584:GLU:O	1:E:597:ARG:HG3	1.82	0.80
2:F:105:ASN:HD21	2:F:127:PRO:CD	1.94	0.80
1:E:267:LEU:HD12	1:E:270:LEU:HD11	1.62	0.79
1:E:492:LEU:HB3	1:E:549:LEU:HD21	1.64	0.79
2:F:240:HIS:HB2	11:G:202:AT5:CM3	2.14	0.78
2:B:242:ILE:HD11	11:C:202:AT5:HM33	1.63	0.78
1:E:320:ARG:HH12	5:E:701:MLI:C2	1.96	0.78
1:E:72:LYS:O	1:E:198:GLU:HA	1.83	0.78
2:F:128:HIS:HD2	2:F:196:TRP:HB3	1.48	0.78
3:G:184:LEU:HB2	3:G:185:PRO:HD2	1.66	0.78
4:H:151:GLU:O	4:H:155:GLU:HG3	1.83	0.78
1:E:383:ILE:HG12	1:E:384:PRO:HD2	1.65	0.78
1:E:522:ASP:O	1:E:525:LYS:HB2	1.83	0.78
1:A:142:ARG:HG2	2:B:168:GLN:O	1.83	0.77
1:A:286:LEU:CD2	6:A:702:FAD:H6	2.13	0.77
3:C:112:ILE:HD13	3:C:117:LEU:HD21	1.65	0.77
1:E:470:GLY:O	1:E:474:ILE:HG22	1.85	0.77
2:B:240:HIS:CB	11:C:202:AT5:HM31	2.15	0.76
1:A:278:THR:HG21	1:A:346:LEU:HD22	1.65	0.76
2:B:88:SER:O	2:B:90:ARG:N	2.19	0.76
3:G:115:VAL:HG23	3:G:116:ILE:HD12	1.68	0.76
1:A:103:PHE:HA	1:A:123:THR:HG21	1.67	0.76
3:C:114:TRP:HB2	3:C:175:ARG:NH1	1.94	0.76
2:F:268:LYS:CG	2:F:269:MET:N	2.46	0.76
1:E:582:GLU:HB2	1:E:603:TRP:CD1	2.20	0.76
2:F:76:LYS:NZ	2:F:83:LEU:O	2.17	0.76
2:F:196:TRP:CZ3	3:G:59:HIS:HB2	2.20	0.76
2:B:40:ILE:HG23	2:B:123:ILE:HB	1.68	0.75
1:E:182:HIS:CE1	2:F:184:LEU:HD22	2.21	0.75
1:E:561:VAL:CG2	1:E:618:ILE:HG21	2.16	0.75
1:A:231:ARG:HD3	1:A:415:GLY:HA2	1.69	0.75
11:C:202:AT5:HM32	11:C:202:AT5:HM23	1.66	0.75
4:H:67:ALA:O	4:H:70:VAL:HG23	1.87	0.74
3:C:49:GLN:OE1	3:C:54:ARG:NH1	2.20	0.74
3:C:82:MET:HB2	10:C:201:HEM:HAC	1.67	0.74
1:E:72:LYS:O	1:E:198:GLU:HG3	1.86	0.74
1:A:320:ARG:HH12	5:A:701:MLI:C2	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LEU:HA	1:A:526:GLU:HG3	1.70	0.73
1:E:83:ALA:HB3	1:E:177:GLY:HA3	1.71	0.73
1:E:432:ARG:HH21	1:E:435:ALA:H	1.35	0.73
1:E:570:ARG:HH11	1:E:581:ARG:HD2	1.52	0.73
3:G:177:GLU:HG3	3:G:181:LYS:HE2	1.70	0.73
1:E:561:VAL:HG21	1:E:618:ILE:CG2	2.18	0.73
1:E:159:ASN:HD22	1:E:163:GLY:HA3	1.53	0.73
1:A:443:VAL:HG12	1:A:444:PHE:CD1	2.24	0.73
1:A:504:ALA:HB2	1:A:560:ILE:HD12	1.71	0.73
3:G:149:ILE:HD13	3:G:149:ILE:N	1.99	0.72
2:B:119:LYS:HA	2:B:119:LYS:HE2	1.70	0.72
2:F:237:PHE:HE2	4:H:59:PHE:CD1	2.07	0.72
2:F:271:THR:HG23	2:F:271:THR:O	1.87	0.72
1:E:88:ASN:O	1:E:439:LEU:HD23	1.89	0.72
1:E:293:GLY:HA2	1:E:317:LEU:HD21	1.71	0.72
1:A:327:GLU:OE2	1:A:384:PRO:HD3	1.89	0.72
2:F:201:LYS:HA	3:G:39:GLN:HG2	1.71	0.72
2:F:128:HIS:CD2	2:F:196:TRP:HB3	2.25	0.71
1:A:503:HIS:CD2	1:A:516:GLY:HA2	2.20	0.71
1:A:159:ASN:O	1:A:162:LYS:HG2	1.91	0.71
2:F:105:ASN:ND2	2:F:127:PRO:HD2	2.04	0.71
1:E:269:ASP:HB3	1:E:272:PHE:HD1	1.56	0.70
1:A:50:GLY:HA3	6:A:702:FAD:O1P	1.91	0.70
3:G:173:TYR:HD2	3:G:174:PRO:HD3	1.54	0.70
1:A:268:GLU:HB3	1:A:608:LEU:HD23	1.73	0.70
2:B:128:HIS:HD2	3:C:59:HIS:CD2	2.10	0.70
2:F:69:LEU:HA	2:F:72:LEU:HD12	1.72	0.70
1:A:77:ARG:HD2	2:B:96:SER:OG	1.92	0.70
4:D:71:PRO:O	4:D:74:PRO:HD2	1.91	0.70
4:H:50:LYS:H	4:H:51:PRO:HD2	1.55	0.69
1:A:52:ALA:N	1:A:441:ALA:HB1	2.08	0.69
1:A:58:MET:HA	1:A:191:CYS:SG	2.32	0.69
1:E:496:MET:HE1	1:E:552:LEU:HB3	1.75	0.69
2:B:230:MET:HE2	2:B:262:ILE:HG21	1.72	0.69
1:A:88:ASN:ND2	1:A:435:ALA:HB3	2.08	0.69
1:E:174:ASP:HB2	1:E:361:PRO:HD2	1.74	0.69
1:E:274:GLN:HB2	1:E:390:MET:HE1	1.72	0.69
2:B:128:HIS:HD2	3:C:59:HIS:HD2	1.41	0.69
2:B:246:THR:OG1	2:B:255:PRO:HD2	1.92	0.69
1:E:496:MET:HG3	1:E:497:GLN:N	2.08	0.69
2:F:149:ILE:HD12	2:F:211:ALA:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:230:MET:HE1	2:F:262:ILE:HG21	1.74	0.69
3:C:112:ILE:H	3:C:112:ILE:HD12	1.57	0.69
2:B:268:LYS:HG2	2:B:269:MET:H	1.58	0.69
3:C:149:ILE:HD13	3:C:149:ILE:N	2.04	0.69
2:B:115:GLN:HA	2:B:115:GLN:HE21	1.58	0.68
4:D:150:PHE:HB3	12:D:201:EPH:H2	1.75	0.68
4:D:109:ARG:HB2	4:D:112:VAL:HG12	1.76	0.68
4:H:50:LYS:N	4:H:51:PRO:CD	2.56	0.68
1:A:401:VAL:HG21	1:A:416:LEU:HG	1.75	0.68
1:E:536:SER:HB2	2:F:46:GLU:CD	2.19	0.68
1:A:286:LEU:HD23	6:A:702:FAD:H6	1.76	0.68
2:B:208:LEU:HD13	2:B:259:ILE:HD11	1.75	0.68
3:G:76:ARG:HE	10:G:201:HEM:CGD	2.07	0.68
10:C:201:HEM:HBD1	10:C:201:HEM:HHA	1.76	0.68
1:E:557:THR:O	1:E:561:VAL:HG13	1.94	0.68
4:H:104:VAL:HG13	4:H:121:VAL:HG12	1.76	0.68
2:B:64:CYS:HB2	2:B:74:LYS:HD2	1.76	0.67
1:E:45:VAL:HG22	1:E:68:ALA:HB3	1.75	0.67
1:E:280:ILE:HG13	1:E:287:ILE:HD11	1.76	0.67
4:H:79:ILE:HD11	4:H:84:MET:HE3	1.76	0.67
2:B:145:GLN:HE22	2:B:195:TYR:HE1	1.43	0.67
3:G:69:TRP:O	3:G:73:GLY:N	2.27	0.67
1:E:113:LEU:HD21	1:E:269:ASP:OD1	1.95	0.67
1:E:360:LEU:HB3	1:E:363:ILE:HD11	1.76	0.67
1:A:476:ASN:O	1:A:480:VAL:HG23	1.94	0.67
1:E:269:ASP:HB3	1:E:272:PHE:CD1	2.31	0.66
1:A:43:ASP:HA	1:A:230:LYS:HE3	1.76	0.66
1:E:508:ARG:HB3	1:E:513:LEU:HD11	1.76	0.66
2:B:129:MET:HE2	2:B:129:MET:HA	1.77	0.66
1:E:40:HIS:O	1:E:228:ARG:HG3	1.96	0.66
1:E:117:ASN:HD22	1:E:117:ASN:H	1.41	0.66
2:B:101:ILE:HG12	2:B:123:ILE:HD12	1.76	0.66
3:C:76:ARG:HE	10:C:201:HEM:CGD	2.07	0.66
1:A:299:VAL:HG13	1:A:303:GLY:HA2	1.78	0.66
1:A:81:THR:HB	1:A:181:LEU:HD23	1.77	0.66
2:B:240:HIS:HB2	11:C:202:AT5:CM3	2.26	0.66
3:C:76:ARG:HA	10:C:201:HEM:O2D	1.96	0.66
3:C:74:LEU:HG	3:C:130:PHE:CE1	2.31	0.66
1:A:286:LEU:HD22	6:A:702:FAD:C6	2.25	0.66
1:A:307:MET:C	1:A:309:ARG:H	2.04	0.66
11:C:202:AT5:HM32	11:C:202:AT5:CM2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:109:ARG:HG2	4:D:109:ARG:NH2	1.95	0.66
1:E:286:LEU:HD23	6:E:702:FAD:H6	1.78	0.65
1:E:502:LYS:HD3	1:E:503:HIS:CE1	2.31	0.65
2:F:202:TYR:CE2	2:F:204:GLY:HA2	2.31	0.65
1:E:140:PHE:HA	1:E:172:VAL:HG22	1.79	0.65
10:C:201:HEM:HHA	10:C:201:HEM:HBA2	1.77	0.65
1:E:215:ILE:HA	1:E:225:HIS:O	1.97	0.65
2:F:254:ASN:CG	2:F:257:ARG:HB2	2.22	0.65
3:G:135:GLY:HA3	10:G:201:HEM:HMB3	1.78	0.65
2:B:127:PRO:HB2	2:B:190:ALA:O	1.96	0.65
4:D:41:ASP:OD1	4:D:44:ALA:HB3	1.96	0.65
1:A:294:GLU:OE2	1:A:359:ARG:HG2	1.96	0.65
2:B:215:ILE:CG2	2:B:226:ARG:HD2	2.26	0.65
1:A:424:CYS:C	1:A:426:SER:H	2.02	0.65
1:A:503:HIS:HE2	1:A:519:LYS:HE2	1.62	0.65
2:F:100:ASN:HD21	2:F:103:GLY:HA2	1.62	0.65
1:E:228:ARG:NH1	1:E:463:PRO:O	2.30	0.65
1:E:395:THR:HA	1:E:400:GLN:O	1.97	0.65
10:G:201:HEM:HBB2	10:G:201:HEM:CMB	2.20	0.65
1:E:52:ALA:H	1:E:441:ALA:HB1	1.61	0.64
1:A:589:LYS:O	1:A:591:ILE:N	2.26	0.64
1:E:583:ASP:O	1:E:602:HIS:HB3	1.97	0.64
2:F:131:VAL:CG2	3:G:55:PRO:HG2	2.21	0.64
2:F:197:TRP:O	4:H:109:ARG:NH2	2.31	0.64
1:E:605:LYS:HD2	1:E:622:TYR:HB3	1.79	0.64
1:A:337:VAL:HG22	1:A:338:GLY:H	1.62	0.64
2:F:230:MET:CE	2:F:262:ILE:HG21	2.28	0.64
4:D:77:TYR:CD1	12:D:201:EPH:H372	2.32	0.64
1:E:383:ILE:HG12	1:E:384:PRO:CD	2.28	0.63
2:F:268:LYS:HG3	2:F:269:MET:N	2.09	0.63
1:A:205:LEU:HB3	1:A:212:VAL:CG2	2.28	0.63
1:A:288:THR:HG23	1:A:291:SER:H	1.61	0.63
1:E:190:ARG:O	4:H:43:ILE:HD11	1.99	0.63
2:B:196:TRP:CZ3	3:C:59:HIS:HB2	2.33	0.63
1:E:174:ASP:CB	1:E:361:PRO:HD2	2.28	0.63
1:E:230:LYS:HE3	1:E:456:LEU:HD11	1.80	0.63
1:E:582:GLU:CB	1:E:603:TRP:HD1	2.11	0.63
1:A:41:ALA:HA	1:A:228:ARG:O	1.98	0.63
2:F:88:SER:O	2:F:90:ARG:N	2.31	0.62
2:F:237:PHE:CE2	4:H:59:PHE:CD1	2.87	0.62
1:A:38:ILE:HD12	1:A:225:HIS:CE1	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:PHE:N	1:A:579:PRO:HD3	2.12	0.62
3:G:36:THR:HB	3:G:37:PRO:HD2	1.81	0.62
1:E:242:ALA:HB2	1:E:552:LEU:HD22	1.81	0.62
1:E:620:LEU:O	1:E:621:ASP:HB2	1.99	0.62
1:A:331:ILE:HG23	1:A:342:ASP:HA	1.80	0.62
1:E:286:LEU:HD23	6:E:702:FAD:C6	2.29	0.62
3:C:133:LEU:O	3:C:136:ILE:HD12	1.99	0.62
3:C:61:THR:HB	3:C:62:ILE:HG23	1.81	0.62
4:H:109:ARG:HG2	4:H:109:ARG:NH2	2.12	0.62
1:A:243:TYR:CG	1:A:386:VAL:HG21	2.35	0.62
1:E:286:LEU:HD12	1:E:287:ILE:N	2.15	0.62
1:A:88:ASN:HD21	1:A:435:ALA:HB3	1.61	0.61
1:A:230:LYS:HD2	1:A:462:ILE:HA	1.82	0.61
1:E:39:ASP:OD2	1:E:226:ARG:NH1	2.33	0.61
1:E:570:ARG:NH1	1:E:581:ARG:CD	2.58	0.61
2:F:89:CYS:HB2	2:F:93:ILE:HG22	1.82	0.61
1:E:437:SER:HB3	6:E:702:FAD:N1	2.15	0.61
4:D:109:ARG:HH21	4:D:109:ARG:CG	2.02	0.61
4:H:44:ALA:HA	4:H:47:LYS:HE2	1.83	0.61
3:C:123:ILE:O	3:C:127:PRO:CD	2.42	0.61
4:D:70:VAL:O	4:D:74:PRO:HD3	2.01	0.61
2:F:129:MET:HE2	2:F:129:MET:HA	1.83	0.61
1:A:72:LYS:HE3	1:A:251:MET:HG3	1.83	0.61
3:C:80:CYS:O	3:C:84:GLY:N	2.32	0.61
3:C:121:LYS:HB3	3:C:171:VAL:HG22	1.83	0.61
1:E:174:ASP:OD2	1:E:362:GLY:N	2.34	0.61
3:G:120:PHE:HA	3:G:123:ILE:HD12	1.83	0.61
2:B:212:TYR:OH	2:B:261:GLU:HG2	2.01	0.61
1:E:39:ASP:HB2	4:H:33:THR:HG22	1.83	0.61
1:E:380:ILE:HG22	1:E:382:VAL:HG13	1.82	0.61
1:A:150:GLN:HA	1:A:169:THR:O	2.01	0.60
3:C:104:VAL:O	3:C:107:ILE:HG13	2.01	0.60
2:F:188:CYS:SG	2:F:206:ALA:HB2	2.42	0.60
1:A:117:ASN:H	1:A:117:ASN:HD22	1.48	0.60
1:E:432:ARG:NH2	1:E:435:ALA:H	2.00	0.60
1:E:526:GLU:C	1:E:528:LYS:H	2.09	0.60
1:A:444:PHE:HA	1:A:447:ALA:HB3	1.82	0.60
2:B:242:ILE:HG23	3:C:69:TRP:HA	1.83	0.60
4:H:58:LEU:O	4:H:61:ILE:HG12	2.02	0.60
1:A:83:ALA:HB3	1:A:177:GLY:CA	2.20	0.60
3:G:112:ILE:CB	3:G:113:PRO:HD3	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:289:GLU:HB2	1:E:320:ARG:NH2	2.16	0.60
3:G:132:THR:HG23	10:G:201:HEM:CBB	2.32	0.60
1:A:233:ILE:HG12	1:A:417:TYR:HB2	1.83	0.59
1:A:325:ARG:NH1	1:A:571:GLY:O	2.35	0.59
2:F:209:MET:HE3	2:F:258:ALA:HB2	1.82	0.59
1:A:276:HIS:HB2	1:A:387:HIS:CB	2.31	0.59
1:A:278:THR:CG2	1:A:346:LEU:HD22	2.32	0.59
2:B:129:MET:HA	2:B:129:MET:CE	2.32	0.59
3:G:175:ARG:O	3:G:175:ARG:HG3	2.02	0.59
1:A:39:ASP:OD1	1:A:226:ARG:NH1	2.35	0.59
2:B:268:LYS:CG	2:B:269:MET:N	2.64	0.59
1:A:628:LYS:H	1:A:628:LYS:HD3	1.66	0.59
2:B:128:HIS:CD2	3:C:59:HIS:HD2	2.20	0.59
2:B:217:ASP:C	2:B:219:ARG:H	2.10	0.59
1:E:231:ARG:HD2	1:E:415:GLY:HA2	1.84	0.59
1:E:562:ALA:HB2	1:E:609:THR:CG2	2.33	0.59
2:F:212:TYR:HB2	2:F:262:ILE:HD11	1.85	0.59
3:G:48:ARG:O	3:G:52:LEU:HG	2.03	0.59
3:G:82:MET:HB2	10:G:201:HEM:HAC	1.84	0.59
1:A:251:MET:HE2	2:B:88:SER:OG	2.02	0.58
2:B:276:LEU:O	2:B:278:THR:N	2.36	0.58
1:E:320:ARG:NH1	5:E:701:MLI:C2	2.66	0.58
1:A:100:LYS:HD3	1:A:635:VAL:HG21	1.85	0.58
1:A:205:LEU:HB2	1:A:213:GLY:O	2.02	0.58
2:B:254:ASN:ND2	3:C:147:THR:O	2.27	0.58
3:C:45:TYR:CE2	3:C:49:GLN:HG3	2.38	0.58
1:E:268:GLU:HG2	1:E:394:PRO:HG3	1.85	0.58
1:E:562:ALA:HB2	1:E:609:THR:HG22	1.84	0.58
2:B:212:TYR:HB2	2:B:262:ILE:HD11	1.84	0.58
1:E:329:ILE:HD11	1:E:507:PHE:HZ	1.68	0.58
1:A:107:ALA:O	1:A:110:SER:OG	2.13	0.58
3:C:82:MET:HG2	12:D:201:EPH:H262	1.85	0.58
1:A:114:GLY:O	1:A:119:MET:HE2	2.04	0.58
1:A:221:ASP:HA	1:A:538:ILE:HG12	1.86	0.58
2:B:243:MET:HE2	3:C:141:PHE:HB3	1.86	0.58
2:B:250:PRO:HD2	8:B:302:SF4:S3	2.44	0.58
2:F:247:LYS:O	2:F:247:LYS:HG3	2.02	0.58
4:H:133:LEU:O	4:H:134:ALA:C	2.45	0.58
1:A:174:ASP:HB2	1:A:361:PRO:HD2	1.85	0.58
1:E:91:LEU:HD23	1:E:127:VAL:HG12	1.86	0.58
1:E:274:GLN:HB2	1:E:390:MET:CE	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:GLY:O	1:E:382:VAL:HA	2.04	0.58
2:B:64:CYS:HB2	2:B:74:LYS:CD	2.34	0.58
3:G:158:LEU:O	3:G:162:LEU:HB2	2.03	0.58
1:A:286:LEU:CD2	6:A:702:FAD:C6	2.82	0.58
1:A:337:VAL:HG11	1:A:345:TYR:CD1	2.38	0.58
1:E:230:LYS:HB3	1:E:456:LEU:HD21	1.86	0.58
1:E:424:CYS:C	1:E:426:SER:N	2.53	0.58
1:A:266:ALA:HB2	1:A:610:LYS:HG2	1.85	0.57
1:A:138:MET:HE1	1:A:180:MET:HB2	1.87	0.57
1:A:333:GLU:HB3	1:A:335:ARG:HH12	1.69	0.57
1:A:503:HIS:NE2	1:A:519:LYS:HE2	2.20	0.57
3:C:126:PHE:HA	3:C:167:SER:OG	2.03	0.57
4:D:71:PRO:C	4:D:74:PRO:HD2	2.29	0.57
1:E:128:GLU:HG2	1:E:446:ARG:HH22	1.69	0.57
2:F:93:ILE:HD13	2:F:93:ILE:O	2.03	0.57
1:A:276:HIS:HB2	1:A:387:HIS:HB2	1.86	0.57
3:C:156:ALA:O	3:C:160:LEU:HB2	2.04	0.57
2:F:254:ASN:OD1	2:F:257:ARG:HB2	2.04	0.57
1:A:231:ARG:CD	1:A:415:GLY:HA2	2.33	0.57
2:B:88:SER:O	2:B:89:CYS:C	2.46	0.57
1:E:203:ASP:O	1:E:215:ILE:HG22	2.05	0.57
1:E:262:ARG:HH22	1:E:551:ASN:HD21	1.52	0.57
4:D:77:TYR:HD1	12:D:201:EPH:H372	1.68	0.57
1:E:213:GLY:HA3	1:E:227:PHE:O	2.05	0.57
1:A:71:THR:OG1	1:A:73:MET:O	2.18	0.57
1:A:432:ARG:NH2	1:A:435:ALA:H	2.02	0.57
3:G:173:TYR:CD2	3:G:174:PRO:HD3	2.38	0.57
1:E:89:ALA:HA	1:E:126:ALA:HB1	1.86	0.57
2:B:47:GLU:HG2	2:B:48:PRO:HD2	1.87	0.56
2:B:237:PHE:HE2	4:D:59:PHE:CD1	2.23	0.56
2:F:262:ILE:HG22	2:F:266:LEU:CD2	2.34	0.56
2:F:268:LYS:HG2	2:F:269:MET:H	1.67	0.56
1:A:281:TYR:HA	1:A:383:ILE:HG22	1.86	0.56
1:A:42:TYR:O	1:A:229:SER:HA	2.05	0.56
5:A:701:MLI:H12	6:A:702:FAD:N5	2.20	0.56
10:C:201:HEM:HBA2	10:C:201:HEM:CHA	2.35	0.56
1:E:71:THR:OG1	6:E:702:FAD:O2B	2.21	0.56
1:E:139:PRO:HA	2:F:219:ARG:HH22	1.69	0.56
2:F:242:ILE:HG12	3:G:72:SER:OG	2.05	0.56
1:E:260:ALA:O	1:E:261:THR:C	2.48	0.56
1:E:432:ARG:HH21	1:E:435:ALA:N	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:517:VAL:O	1:E:521:MET:HG2	2.06	0.56
1:E:590:PRO:C	1:E:592:GLU:H	2.13	0.56
1:A:65:PHE:HE2	1:A:456:LEU:HD12	1.69	0.56
1:A:434:GLY:O	1:A:435:ALA:HB3	2.06	0.56
2:B:35:ILE:HG22	2:B:58:ASP:HB3	1.86	0.56
1:E:249:ALA:HB1	2:F:88:SER:OG	2.05	0.56
3:G:134:ASN:O	3:G:137:ARG:HB3	2.05	0.56
4:H:69:MET:O	4:H:73:ILE:HD12	2.06	0.56
2:B:242:ILE:CD1	11:C:202:AT5:HM33	2.35	0.56
3:C:133:LEU:HA	3:C:136:ILE:HD11	1.86	0.56
1:E:157:SER:HA	1:E:166:ALA:HB2	1.87	0.56
4:H:131:CYS:O	4:H:132:LEU:C	2.49	0.56
1:E:42:TYR:O	1:E:229:SER:HA	2.06	0.56
1:E:43:ASP:O	1:E:230:LYS:HB2	2.05	0.56
3:G:73:GLY:HA2	11:G:202:AT5:O4	2.06	0.56
3:G:173:TYR:C	3:G:175:ARG:H	2.13	0.56
2:F:92:GLY:HA2	2:F:109:CYS:SG	2.45	0.56
1:A:83:ALA:HA	6:A:702:FAD:N5	2.21	0.56
1:A:172:VAL:HG21	1:A:179:SER:HB3	1.88	0.56
1:E:243:TYR:HB3	1:E:501:GLN:OE1	2.06	0.56
3:G:50:ARG:HG3	3:G:51:ALA:N	2.21	0.56
2:B:230:MET:CE	2:B:262:ILE:HG21	2.35	0.56
4:D:97:HIS:HB2	4:D:129:THR:HG23	1.87	0.56
2:F:195:TYR:O	2:F:199:ALA:HB2	2.05	0.56
1:A:193:CYS:O	1:A:194:THR:C	2.48	0.55
2:B:230:MET:HB2	2:B:236:ALA:HB2	1.88	0.55
2:F:55:GLN:HB3	2:F:57:PHE:HE1	1.70	0.55
1:A:83:ALA:CB	1:A:438:LEU:HD21	2.37	0.55
1:A:151:ARG:HG3	1:A:169:THR:HB	1.89	0.55
1:A:174:ASP:OD1	1:A:174:ASP:O	2.24	0.55
1:A:289:GLU:HB3	5:A:701:MLI:O9	2.05	0.55
1:A:204:LEU:HD22	1:A:211:CYS:SG	2.47	0.55
1:A:489:THR:HG21	1:A:542:ASP:OD1	2.06	0.55
2:B:231:GLN:HB3	4:D:54:SER:HA	1.88	0.55
1:E:112:TRP:CE2	1:E:640:PRO:HA	2.41	0.55
3:G:82:MET:HE3	10:G:201:HEM:CAC	2.34	0.55
1:A:452:ILE:C	1:A:454:GLU:H	2.14	0.55
2:F:146:TYR:O	2:F:149:ILE:HG12	2.06	0.55
3:G:184:LEU:HB2	3:G:185:PRO:CD	2.36	0.55
1:A:138:MET:CE	1:A:180:MET:HB2	2.36	0.55
2:B:105:ASN:HD21	2:B:127:PRO:CD	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:PHE:CZ	1:E:289:GLU:HB3	2.42	0.55
1:A:274:GLN:CB	1:A:390:MET:HE1	2.34	0.55
2:F:245:CYS:HB2	2:F:255:PRO:HG2	1.89	0.55
2:B:160:ASN:HB3	2:B:163:GLU:HB2	1.89	0.55
1:E:146:GLY:HA3	2:F:167:TYR:CE1	2.42	0.55
2:B:264:MET:SD	3:C:143:MET:HG2	2.47	0.54
4:D:97:HIS:HB2	4:D:129:THR:CG2	2.38	0.54
3:G:100:PHE:O	3:G:103:PHE:HB3	2.06	0.54
1:E:346:LEU:HB2	1:E:382:VAL:HG21	1.90	0.54
2:F:240:HIS:O	2:F:241:THR:HG23	2.07	0.54
1:A:147:LYS:HA	2:B:165:GLN:NE2	2.22	0.54
1:A:206:MET:HG3	1:A:263:ALA:HB1	1.89	0.54
1:A:268:GLU:HA	1:A:607:THR:O	2.08	0.54
1:A:370:PHE:CZ	2:B:110:ILE:HG22	2.42	0.54
1:E:570:ARG:HG3	1:E:581:ARG:HD2	1.89	0.54
1:A:388:TYR:HE1	1:A:437:SER:HG	1.56	0.54
2:B:181:GLU:O	2:B:182:CYS:C	2.50	0.54
1:E:102:HIS:CE1	1:E:123:THR:HG22	2.42	0.54
1:E:286:LEU:HD22	1:E:387:HIS:CE1	2.42	0.54
1:A:586:ASP:OD1	1:A:588:SER:OG	2.24	0.54
1:E:471:GLU:HA	1:E:474:ILE:CG2	2.38	0.54
1:E:602:HIS:O	1:E:605:LYS:HE2	2.08	0.54
3:G:42:GLY:O	3:G:45:TYR:HB3	2.07	0.54
1:A:393:ILE:HG22	1:A:401:VAL:HG13	1.90	0.54
2:B:215:ILE:HG22	2:B:226:ARG:HD2	1.89	0.54
2:F:241:THR:O	2:F:241:THR:OG1	2.25	0.54
4:H:66:ALA:HA	4:H:69:MET:HG3	1.90	0.54
1:A:394:PRO:O	1:A:401:VAL:HA	2.07	0.54
3:C:82:MET:CB	10:C:201:HEM:HAC	2.36	0.53
3:G:148:ASP:OD2	3:G:150:PRO:HD2	2.08	0.53
3:C:91:VAL:O	3:C:92:GLY:C	2.50	0.53
1:A:500:MET:HE1	1:A:556:ALA:O	2.08	0.53
1:A:142:ARG:HB3	2:B:170:ILE:HG22	1.90	0.53
1:E:394:PRO:O	1:E:401:VAL:HA	2.08	0.53
1:A:41:ALA:HB1	1:A:462:ILE:HG21	1.89	0.53
1:A:226:ARG:HH21	1:A:469:ALA:HB3	1.74	0.53
1:A:605:LYS:HA	1:A:625:VAL:HG23	1.89	0.53
1:E:172:VAL:O	1:E:173:ALA:HB3	2.08	0.53
1:E:220:GLU:OE2	3:G:54:ARG:NH2	2.41	0.53
2:B:188:CYS:O	2:B:191:SER:OG	2.19	0.53
1:E:561:VAL:HG23	1:E:620:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:CYS:C	1:A:426:SER:N	2.67	0.53
2:B:237:PHE:CE2	4:D:59:PHE:CD1	2.97	0.53
2:F:240:HIS:C	2:F:241:THR:CG2	2.82	0.53
2:F:261:GLU:OE2	2:F:269:MET:HE1	2.07	0.53
4:H:50:LYS:H	4:H:51:PRO:CD	2.19	0.53
1:A:394:PRO:HB2	1:A:402:ILE:HG13	1.90	0.53
4:H:85:ASP:OD1	4:H:145:GLY:HA3	2.09	0.53
1:A:537:LEU:O	1:A:538:ILE:C	2.51	0.53
1:A:98:ASP:OD2	1:A:100:LYS:HG3	2.09	0.52
2:B:100:ASN:N	2:B:124:TYR:O	2.36	0.52
2:F:242:ILE:HD11	11:G:202:AT5:HM33	1.90	0.52
2:B:201:LYS:HA	3:C:39:GLN:HG2	1.92	0.52
2:B:205:PRO:O	2:B:206:ALA:C	2.51	0.52
2:B:245:CYS:SG	2:B:255:PRO:HG2	2.49	0.52
1:E:80:THR:HG22	1:E:181:LEU:HB2	1.90	0.52
1:E:585:TYR:N	1:E:585:TYR:HD1	2.07	0.52
3:C:50:ARG:HG3	3:C:51:ALA:N	2.23	0.52
3:C:112:ILE:HD12	3:C:112:ILE:N	2.24	0.52
10:C:201:HEM:HBB2	10:C:201:HEM:CMB	2.31	0.52
1:E:363:ILE:O	1:E:364:SER:C	2.52	0.52
1:E:391:GLY:HA2	1:E:424:CYS:SG	2.49	0.52
1:A:119:MET:O	1:A:123:THR:HG23	2.09	0.52
4:H:28:THR:O	4:H:30:ALA:N	2.41	0.52
1:A:294:GLU:CD	1:A:359:ARG:HG2	2.35	0.52
2:B:188:CYS:SG	2:B:206:ALA:HB2	2.50	0.52
1:E:427:VAL:HG11	1:E:444:PHE:CE1	2.44	0.52
1:E:523:LEU:C	1:E:525:LYS:N	2.65	0.52
1:A:172:VAL:HG21	1:A:179:SER:CB	2.40	0.52
1:E:606:HIS:HD2	1:E:623:ARG:NH1	2.08	0.52
3:G:58:PRO:HB2	3:G:62:ILE:HG12	1.92	0.52
1:A:76:THR:CG2	1:A:76:THR:O	2.58	0.52
1:E:307:MET:HE2	1:E:323:VAL:HG22	1.91	0.52
1:E:355:GLN:O	1:E:359:ARG:HB2	2.10	0.52
1:E:363:ILE:HG13	1:E:364:SER:H	1.73	0.52
1:E:598:PRO:HD2	1:E:601:LYS:HB2	1.91	0.52
2:F:148:SER:HB3	3:G:38:ILE:HD13	1.92	0.52
2:F:179:LEU:HD23	2:F:213:ARG:HA	1.92	0.52
4:D:43:ILE:O	4:D:46:GLU:HB3	2.09	0.52
1:E:428:HIS:HB3	1:E:432:ARG:CA	2.38	0.52
1:A:83:ALA:HA	6:A:702:FAD:C5X	2.40	0.51
2:B:254:ASN:OD1	2:B:257:ARG:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:476:ASN:O	1:E:480:VAL:HG23	2.09	0.51
4:D:109:ARG:O	4:D:113:LEU:HB2	2.10	0.51
1:E:74:PHE:O	1:E:76:THR:N	2.43	0.51
1:E:268:GLU:OE1	1:E:394:PRO:HB3	2.10	0.51
2:F:271:THR:O	2:F:271:THR:CG2	2.58	0.51
4:H:67:ALA:C	4:H:69:MET:N	2.68	0.51
2:B:34:ARG:HB2	2:B:117:THR:HG21	1.92	0.51
3:C:132:THR:HG23	10:C:201:HEM:CAB	2.41	0.51
11:C:202:AT5:H12	4:D:107:TYR:OH	2.10	0.51
2:F:261:GLU:O	2:F:265:LEU:HD12	2.10	0.51
4:H:59:PHE:O	4:H:60:LYS:C	2.53	0.51
1:A:523:LEU:C	1:A:525:LYS:H	2.19	0.51
1:E:95:ASN:HD21	1:E:167:LYS:HB2	1.75	0.51
1:E:233:ILE:HA	1:E:417:TYR:O	2.09	0.51
1:E:262:ARG:HH22	1:E:551:ASN:ND2	2.08	0.51
1:E:265:ILE:HD12	1:E:401:VAL:HG11	1.93	0.51
1:A:73:MET:HE3	1:A:78:SER:HA	1.92	0.51
1:A:87:ILE:HD11	1:A:439:LEU:HA	1.92	0.51
1:A:257:THR:HG22	1:A:267:LEU:HD22	1.92	0.51
3:C:121:LYS:HE2	4:D:154:TRP:HA	1.93	0.51
2:B:102:ALA:HA	2:B:122:LYS:HZ3	1.76	0.51
1:E:102:HIS:ND1	1:E:123:THR:HG22	2.25	0.51
4:H:54:SER:C	4:H:56:GLY:H	2.18	0.51
1:E:104:TYR:CD2	1:E:160:TYR:HA	2.45	0.51
4:H:43:ILE:O	4:H:46:GLU:HB3	2.11	0.51
2:F:240:HIS:CG	11:G:202:AT5:HM31	2.45	0.51
1:A:307:MET:C	1:A:309:ARG:N	2.69	0.51
1:A:517:VAL:HG22	1:A:560:ILE:HG23	1.93	0.51
3:C:112:ILE:CD1	3:C:117:LEU:HD21	2.38	0.51
1:E:134:GLU:HG3	1:E:148:ILE:HD11	1.93	0.51
2:F:57:PHE:HD2	2:F:75:ILE:HD12	1.73	0.51
4:H:146:LEU:O	4:H:149:ALA:HB3	2.09	0.51
3:C:133:LEU:HB3	3:C:159:VAL:HG13	1.92	0.51
3:C:173:TYR:O	3:C:176:TRP:HB3	2.11	0.51
1:E:544:THR:C	1:E:546:SER:N	2.68	0.51
1:A:86:GLY:O	1:A:438:LEU:HD12	2.11	0.50
1:A:113:LEU:HD21	1:A:269:ASP:OD1	2.12	0.50
1:A:513:LEU:HD13	1:A:564:GLU:HA	1.92	0.50
1:A:538:ILE:O	1:A:539:TRP:C	2.55	0.50
2:B:258:ALA:O	2:B:259:ILE:C	2.53	0.50
1:E:321:ASP:OD2	1:E:571:GLY:HA2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:331:ILE:HD11	1:E:344:ILE:HG23	1.92	0.50
1:A:345:TYR:CD2	1:A:379:PRO:HG2	2.46	0.50
2:B:85:PHE:CD1	2:B:85:PHE:N	2.79	0.50
3:C:112:ILE:HG22	3:C:113:PRO:HD2	1.93	0.50
1:E:157:SER:HB2	1:E:164:GLY:O	2.11	0.50
1:E:428:HIS:ND1	1:E:432:ARG:HG3	2.26	0.50
1:E:214:VAL:HG12	1:E:215:ILE:N	2.27	0.50
2:B:126:LEU:HD22	2:B:190:ALA:HB3	1.92	0.50
2:F:36:LYS:HD2	2:F:37:THR:H	1.77	0.50
4:D:58:LEU:HD23	4:D:58:LEU:O	2.12	0.50
1:E:45:VAL:CG2	1:E:68:ALA:HB3	2.41	0.50
2:F:213:ARG:HD3	2:F:213:ARG:C	2.37	0.50
1:A:126:ALA:CB	1:A:439:LEU:HD21	2.42	0.50
1:A:439:LEU:O	1:A:443:VAL:HB	2.12	0.50
2:B:181:GLU:HB2	2:B:253:LEU:HD21	1.94	0.50
2:B:217:ASP:C	2:B:219:ARG:N	2.70	0.50
1:E:585:TYR:N	1:E:585:TYR:CD1	2.79	0.50
1:A:383:ILE:HG12	1:A:384:PRO:O	2.12	0.50
2:B:139:MET:HB3	2:B:143:TYR:CE2	2.47	0.50
1:E:99:TRP:CE3	1:E:99:TRP:C	2.90	0.50
3:G:169:ALA:O	3:G:173:TYR:HB3	2.12	0.50
4:H:67:ALA:O	4:H:69:MET:N	2.45	0.50
1:E:186:GLY:O	1:E:189:LEU:HB2	2.11	0.50
1:E:526:GLU:C	1:E:528:LYS:N	2.70	0.50
1:A:37:VAL:HG21	4:D:29:SER:HA	1.92	0.49
1:A:73:MET:CE	1:A:78:SER:HA	2.42	0.49
2:B:89:CYS:SG	2:B:90:ARG:N	2.84	0.49
2:F:242:ILE:HD11	11:G:202:AT5:CM3	2.42	0.49
1:A:58:MET:HE1	1:A:187:ASN:CB	2.42	0.49
1:E:78:SER:OG	6:E:702:FAD:O3B	2.19	0.49
1:E:390:MET:O	1:E:391:GLY:O	2.30	0.49
1:A:432:ARG:HH21	1:A:435:ALA:H	1.61	0.49
1:A:443:VAL:HG12	1:A:444:PHE:HD1	1.75	0.49
3:C:59:HIS:O	3:C:62:ILE:HG13	2.12	0.49
1:E:249:ALA:C	1:E:251:MET:H	2.19	0.49
2:F:212:TYR:HA	2:F:215:ILE:HG12	1.93	0.49
3:G:86:LEU:HB2	4:H:132:LEU:HD11	1.94	0.49
2:B:125:PRO:O	2:B:126:LEU:C	2.55	0.49
3:C:148:ASP:OD2	3:C:150:PRO:HD2	2.13	0.49
4:D:101:TRP:CH2	4:D:122:ARG:HG2	2.48	0.49
3:C:149:ILE:HG12	3:C:150:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:201:HEM:NC	4:D:95:HIS:CD2	2.80	0.49
4:H:129:THR:O	4:H:130:ALA:C	2.55	0.49
2:B:268:LYS:NZ	3:C:143:MET:HE2	2.27	0.49
2:F:240:HIS:C	2:F:241:THR:HG23	2.37	0.49
4:H:77:TYR:HA	12:H:201:EPH:H11	1.93	0.49
1:A:148:ILE:H	2:B:165:GLN:NE2	2.10	0.49
1:A:307:MET:HE2	1:A:323:VAL:HG22	1.95	0.49
1:E:43:ASP:HA	1:E:230:LYS:HD3	1.95	0.49
2:F:124:TYR:HB3	2:F:125:PRO:CD	2.43	0.49
4:H:140:ASN:HA	4:H:145:GLY:HA2	1.94	0.49
1:A:43:ASP:H	1:A:66:LYS:HB3	1.77	0.49
1:A:74:PHE:HA	1:A:197:ILE:HG23	1.93	0.49
1:A:93:SER:HB3	1:A:147:LYS:CB	2.43	0.49
1:A:331:ILE:HD11	1:A:344:ILE:HG22	1.95	0.49
1:A:276:HIS:O	1:A:384:PRO:HA	2.13	0.49
1:A:470:GLY:O	1:A:473:SER:HB2	2.12	0.49
1:E:49:ALA:HB1	1:E:75:PRO:HB3	1.95	0.49
1:E:325:ARG:O	1:E:326:ALA:C	2.56	0.49
11:G:202:AT5:O1	11:G:202:AT5:H111	2.12	0.49
1:A:567:LYS:HB3	1:A:578:PHE:CE1	2.47	0.48
2:B:35:ILE:CG2	2:B:58:ASP:HB3	2.43	0.48
2:B:39:GLU:HA	2:B:55:GLN:O	2.13	0.48
1:E:113:LEU:O	1:E:606:HIS:HE1	1.96	0.48
1:E:120:HIS:CD2	1:E:630:LEU:HB2	2.48	0.48
2:F:66:THR:HG23	2:F:67:MET:HG2	1.94	0.48
2:F:197:TRP:HA	4:H:109:ARG:NH2	2.28	0.48
3:C:88:ILE:O	3:C:92:GLY:HA3	2.13	0.48
3:C:136:ILE:HA	3:C:139:ILE:HD12	1.95	0.48
1:E:77:ARG:HD2	2:F:96:SER:OG	2.13	0.48
1:E:241:ARG:HA	1:E:241:ARG:HD3	1.58	0.48
1:E:268:GLU:HB3	1:E:608:LEU:HD22	1.96	0.48
1:E:584:GLU:C	1:E:585:TYR:HD1	2.21	0.48
2:F:168:GLN:NE2	2:F:173:GLN:HA	2.27	0.48
3:G:71:VAL:HG11	3:G:137:ARG:NH1	2.28	0.48
1:A:142:ARG:CG	2:B:168:GLN:O	2.59	0.48
1:E:109:GLY:O	1:E:431:ASN:HB3	2.14	0.48
1:E:508:ARG:HH11	1:E:573:HIS:HA	1.78	0.48
1:A:38:ILE:N	1:A:224:ILE:O	2.45	0.48
2:B:242:ILE:O	2:B:243:MET:HB2	2.13	0.48
3:C:107:ILE:HD11	4:D:156:LEU:CD2	2.25	0.48
3:G:175:ARG:HH22	3:G:178:ARG:NH2	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:67:ALA:C	4:H:69:MET:H	2.22	0.48
1:A:55:ARG:HG2	1:A:442:VAL:O	2.14	0.48
1:A:320:ARG:H	1:A:320:ARG:HG2	1.33	0.48
3:C:76:ARG:NH1	4:D:107:TYR:HE1	2.11	0.48
4:D:131:CYS:O	4:D:132:LEU:C	2.56	0.48
1:E:139:PRO:HA	2:F:219:ARG:NH2	2.28	0.48
1:E:618:ILE:HG22	1:E:620:LEU:HD12	1.96	0.48
3:G:116:ILE:HA	3:G:119:THR:HB	1.96	0.48
1:A:58:MET:CE	1:A:187:ASN:HB3	2.43	0.48
1:A:76:THR:HG23	1:A:182:HIS:NE2	2.29	0.48
1:A:416:LEU:C	1:A:417:TYR:HD1	2.21	0.48
3:C:60:LEU:HD22	11:C:202:AT5:C10	2.42	0.48
1:E:253:THR:HG21	1:E:548:GLU:HB3	1.95	0.48
1:E:438:LEU:O	1:E:441:ALA:N	2.47	0.48
3:C:132:THR:HG21	4:D:73:ILE:HG21	1.96	0.48
2:B:231:GLN:OE1	4:D:52:LEU:HG	2.13	0.48
2:B:268:LYS:HE2	2:B:268:LYS:HB3	1.37	0.48
1:E:555:ASN:O	1:E:559:THR:OG1	2.26	0.48
5:E:701:MLI:H12	6:E:702:FAD:N5	2.29	0.48
3:G:107:ILE:HG13	3:G:108:ARG:N	2.28	0.48
3:C:105:GLU:C	3:C:107:ILE:H	2.21	0.48
1:E:79:HIS:HD2	6:E:702:FAD:HM83	1.68	0.48
1:E:103:PHE:HA	1:E:123:THR:HG21	1.96	0.48
1:E:241:ARG:C	1:E:243:TYR:H	2.22	0.48
2:F:149:ILE:O	2:F:150:GLN:HB2	2.12	0.48
1:A:549:LEU:HD12	1:A:549:LEU:O	2.14	0.48
1:A:558:GLN:NE2	1:A:611:GLN:HB3	2.29	0.48
2:B:128:HIS:CD2	3:C:59:HIS:CD2	2.97	0.48
2:B:142:PHE:HE1	2:B:206:ALA:HB3	1.78	0.48
2:B:268:LYS:HG2	2:B:269:MET:N	2.24	0.48
1:E:427:VAL:HG23	1:E:428:HIS:CD2	2.48	0.48
2:F:129:MET:HA	2:F:129:MET:CE	2.44	0.48
3:C:86:LEU:HB2	4:D:132:LEU:HD11	1.96	0.47
1:E:275:PHE:CE2	1:E:386:VAL:HG23	2.49	0.47
4:H:92:LEU:O	4:H:93:THR:C	2.57	0.47
1:A:496:MET:CG	1:A:497:GLN:N	2.77	0.47
2:B:44:ASN:HD22	2:B:47:GLU:HB2	1.79	0.47
4:D:100:VAL:O	4:D:104:VAL:HB	2.14	0.47
1:A:325:ARG:HG2	1:A:506:VAL:HG12	1.96	0.47
1:A:508:ARG:NH1	1:A:573:HIS:HA	2.29	0.47
1:A:545:GLU:HA	1:A:548:GLU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:GLU:OE2	3:C:34:GLU:HA	2.13	0.47
1:E:138:MET:HE3	1:E:180:MET:H	1.79	0.47
2:F:101:ILE:HG21	2:F:111:CYS:SG	2.54	0.47
2:B:86:ARG:HD2	2:B:136:VAL:HG13	1.95	0.47
3:C:129:ALA:O	3:C:133:LEU:HD22	2.13	0.47
1:E:99:TRP:HE3	1:E:99:TRP:O	1.96	0.47
1:E:554:LEU:HD22	1:E:611:GLN:OE1	2.14	0.47
3:G:80:CYS:O	3:G:81:ALA:C	2.57	0.47
1:A:47:ILE:CG2	1:A:201:ALA:HB2	2.45	0.47
2:F:172:GLU:OE2	2:F:275:PRO:HD2	2.14	0.47
3:G:135:GLY:HA3	10:G:201:HEM:CMB	2.44	0.47
2:B:146:TYR:HA	2:B:207:VAL:HG13	1.97	0.47
2:B:201:LYS:O	2:B:235:SER:HA	2.14	0.47
1:E:117:ASN:HD22	1:E:117:ASN:N	2.09	0.47
1:E:214:VAL:CG2	1:E:232:THR:HG21	2.45	0.47
2:B:234:PHE:O	2:B:238:LYS:HB2	2.15	0.47
3:C:66:GLN:HB2	3:C:69:TRP:CD1	2.49	0.47
4:D:84:MET:HE3	4:D:84:MET:HA	1.96	0.47
1:E:289:GLU:CD	1:E:320:ARG:HH21	2.23	0.47
1:E:603:TRP:O	1:E:605:LYS:N	2.44	0.47
2:F:235:SER:HB3	3:G:39:GLN:NE2	2.30	0.47
1:A:503:HIS:CD2	1:A:516:GLY:CA	2.81	0.47
1:A:482:TYR:O	1:A:483:ALA:C	2.58	0.47
2:B:69:LEU:HD12	2:B:109:CYS:CB	2.45	0.47
3:G:97:PRO:HG2	3:G:98:LEU:H	1.79	0.47
10:G:201:HEM:HMB1	10:G:201:HEM:CBB	2.27	0.47
1:A:452:ILE:C	1:A:454:GLU:N	2.73	0.47
2:B:185:CYS:SG	8:B:302:SF4:S3	3.12	0.47
3:C:60:LEU:HD22	11:C:202:AT5:H101	1.97	0.47
1:E:585:TYR:HE1	1:E:596:LYS:HD3	1.80	0.47
4:H:93:THR:HA	4:H:132:LEU:HD23	1.96	0.47
4:H:105:ASN:HA	4:H:122:ARG:HH12	1.79	0.47
1:A:58:MET:HE1	1:A:187:ASN:HB3	1.96	0.46
2:B:141:LEU:HB2	3:C:45:TYR:CE1	2.51	0.46
3:C:114:TRP:CD1	3:C:175:ARG:HE	2.33	0.46
1:A:102:HIS:O	1:A:106:THR:OG1	2.27	0.46
1:A:331:ILE:HD11	1:A:344:ILE:CG2	2.46	0.46
1:A:385:THR:O	1:A:386:VAL:C	2.58	0.46
1:A:493:ARG:HB2	1:A:549:LEU:HD22	1.97	0.46
3:C:133:LEU:HA	3:C:133:LEU:HD12	1.75	0.46
4:D:54:SER:C	4:D:56:GLY:H	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:MET:HA	1:E:191:CYS:SG	2.56	0.46
1:E:60:LEU:HD21	1:E:449:SER:HA	1.97	0.46
1:E:103:PHE:CE2	1:E:638:ILE:HD11	2.50	0.46
2:F:36:LYS:HB2	2:F:61:LEU:CD1	2.46	0.46
2:F:156:LYS:HB3	2:F:156:LYS:HE2	1.67	0.46
1:A:457:LYS:O	1:A:459:ASP:N	2.48	0.46
1:E:613:PRO:HG2	1:E:614:ARG:HH11	1.81	0.46
3:G:173:TYR:C	3:G:175:ARG:N	2.74	0.46
4:H:133:LEU:O	4:H:136:LEU:N	2.48	0.46
1:A:111:ASP:O	1:A:570:ARG:HD3	2.16	0.46
1:A:333:GLU:O	1:A:335:ARG:NH1	2.48	0.46
2:B:222:SER:O	2:B:223:ALA:C	2.58	0.46
1:E:142:ARG:HB2	2:F:173:GLN:HG2	1.97	0.46
2:F:125:PRO:O	2:F:126:LEU:C	2.58	0.46
11:G:202:AT5:H111	11:G:202:AT5:C1	2.45	0.46
1:A:153:PHE:HB2	1:A:169:THR:OG1	2.15	0.46
3:C:118:ASP:O	3:C:171:VAL:HG11	2.16	0.46
1:E:34:GLN:OE1	1:E:34:GLN:HA	2.16	0.46
1:E:107:ALA:HA	1:E:119:MET:HE1	1.98	0.46
1:E:182:HIS:ND1	2:F:184:LEU:HD22	2.30	0.46
1:E:202:LEU:HD11	1:E:477:LEU:HD13	1.97	0.46
1:E:245:SER:OG	1:E:385:THR:HG21	2.15	0.46
4:H:108:GLY:O	4:H:122:ARG:NH2	2.48	0.46
1:E:52:ALA:N	1:E:441:ALA:HB1	2.30	0.46
4:H:153:VAL:C	4:H:155:GLU:H	2.24	0.46
2:B:86:ARG:HH12	2:B:139:MET:HB2	1.81	0.46
1:E:73:MET:HB3	1:E:251:MET:HE3	1.97	0.46
1:E:77:ARG:HA	2:F:94:CYS:HB2	1.97	0.46
1:E:139:PRO:HB3	2:F:176:LEU:HD23	1.97	0.46
1:E:298:LEU:HB3	1:E:306:PHE:CE2	2.51	0.46
1:A:276:HIS:CE1	1:A:286:LEU:CD1	2.99	0.46
2:F:238:LYS:O	2:F:240:HIS:CD2	2.69	0.46
2:F:242:ILE:HB	9:F:303:F3S:S4	2.55	0.46
3:G:122:PHE:HA	3:G:171:VAL:HG21	1.97	0.46
2:B:181:GLU:CD	2:B:181:GLU:H	2.23	0.46
3:C:135:GLY:O	3:C:136:ILE:C	2.59	0.46
1:E:231:ARG:HA	1:E:231:ARG:HD3	1.55	0.46
1:E:363:ILE:HG13	1:E:364:SER:N	2.31	0.46
2:F:68:VAL:O	2:F:69:LEU:C	2.57	0.46
2:F:230:MET:HE1	2:F:262:ILE:HD13	1.98	0.46
2:B:89:CYS:HB2	2:B:93:ILE:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:LEU:HB3	2:B:190:ALA:CB	2.45	0.46
1:E:496:MET:O	1:E:500:MET:HB2	2.15	0.46
4:H:50:LYS:O	4:H:51:PRO:C	2.59	0.46
1:A:120:HIS:HD2	1:A:630:LEU:H	1.64	0.45
1:A:390:MET:SD	1:A:432:ARG:HB2	2.56	0.45
2:B:215:ILE:HG23	2:B:226:ARG:HD2	1.97	0.45
1:E:361:PRO:HG2	1:E:362:GLY:H	1.80	0.45
1:A:268:GLU:HB3	1:A:608:LEU:CD2	2.43	0.45
1:E:159:ASN:O	1:E:160:TYR:C	2.60	0.45
2:F:36:LYS:HB2	2:F:61:LEU:HD12	1.98	0.45
2:F:181:GLU:O	2:F:182:CYS:C	2.60	0.45
1:A:47:ILE:HG21	1:A:201:ALA:CB	2.46	0.45
1:A:74:PHE:HA	1:A:197:ILE:CG2	2.46	0.45
2:B:214:TRP:HB3	2:B:226:ARG:CZ	2.45	0.45
4:D:101:TRP:CZ3	4:D:122:ARG:HG2	2.51	0.45
1:E:46:ILE:HG12	1:E:233:ILE:HD12	1.99	0.45
1:E:241:ARG:HH22	2:F:90:ARG:HH12	1.64	0.45
1:E:246:CYS:HA	1:E:386:VAL:O	2.16	0.45
3:G:171:VAL:HA	4:H:154:TRP:HE1	1.80	0.45
1:A:98:ASP:C	1:A:100:LYS:H	2.24	0.45
1:A:360:LEU:N	1:A:361:PRO:CD	2.79	0.45
1:E:514:ALA:HA	1:E:517:VAL:HG23	1.97	0.45
1:E:612:ASP:HB3	1:E:616:GLY:H	1.82	0.45
4:H:85:ASP:CG	4:H:146:LEU:H	2.24	0.45
1:A:121:TYR:CE1	1:A:447:ALA:HB2	2.51	0.45
1:A:276:HIS:HB2	1:A:387:HIS:CG	2.51	0.45
1:A:337:VAL:CG1	1:A:345:TYR:CD1	2.99	0.45
10:C:201:HEM:HBB1	4:D:70:VAL:HA	1.98	0.45
1:E:374:ASP:OD1	1:E:374:ASP:C	2.60	0.45
1:E:516:GLY:O	1:E:517:VAL:C	2.59	0.45
2:F:257:ARG:HG2	3:G:147:THR:OG1	2.16	0.45
1:E:280:ILE:CG1	1:E:287:ILE:HD11	2.46	0.45
4:H:93:THR:HG21	4:H:133:LEU:HB2	1.98	0.45
2:B:47:GLU:OE2	2:B:48:PRO:O	2.35	0.45
2:B:76:LYS:HA	2:B:80:ASP:O	2.16	0.45
1:E:122:LEU:HA	1:E:443:VAL:HG11	1.98	0.45
1:A:246:CYS:O	2:B:90:ARG:NH2	2.50	0.45
1:A:481:ARG:NH2	1:A:537:LEU:HG	2.32	0.45
1:E:514:ALA:HB2	1:E:564:GLU:HG3	1.99	0.45
3:G:52:LEU:HD12	3:G:54:ARG:NH1	2.31	0.45
1:A:277:PRO:HA	1:A:324:SER:OG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:ILE:HA	1:A:639:PRO:HD3	1.85	0.45
2:B:242:ILE:HD11	11:C:202:AT5:CM3	2.43	0.45
1:E:353:ALA:HB2	1:E:376:THR:HG21	1.97	0.45
1:E:437:SER:OG	6:E:702:FAD:H2'	2.17	0.45
1:E:635:VAL:HG22	1:E:636:ASP:H	1.80	0.45
2:F:89:CYS:SG	2:F:90:ARG:N	2.90	0.45
2:F:136:VAL:HA	2:F:137:PRO:HD3	1.64	0.45
1:A:196:PHE:O	1:A:199:TYR:CD1	2.70	0.45
1:A:628:LYS:H	1:A:628:LYS:CD	2.29	0.45
2:B:249:CYS:HA	8:B:302:SF4:S3	2.57	0.45
4:D:140:ASN:N	4:D:140:ASN:ND2	2.62	0.45
1:E:275:PHE:CE1	1:E:506:VAL:HA	2.52	0.45
1:E:388:TYR:CD2	1:E:432:ARG:HD2	2.52	0.45
1:A:78:SER:O	1:A:81:THR:HG22	2.17	0.44
3:C:152:ILE:HG22	3:C:153:TYR:N	2.31	0.44
1:A:642:ILE:H	1:A:642:ILE:HG13	1.53	0.44
2:B:131:VAL:O	3:C:54:ARG:HD3	2.18	0.44
2:F:268:LYS:HE2	2:F:268:LYS:HB3	1.65	0.44
1:A:495:THR:O	1:A:499:THR:HG23	2.18	0.44
2:B:194:SER:HB3	2:B:202:TYR:CD2	2.52	0.44
2:F:100:ASN:HD21	2:F:103:GLY:CA	2.28	0.44
2:F:115:GLN:HE21	2:F:115:GLN:CA	2.05	0.44
1:A:325:ARG:HG2	1:A:506:VAL:CG1	2.48	0.44
1:A:600:GLU:N	1:A:600:GLU:OE2	2.51	0.44
1:A:635:VAL:HG22	1:A:636:ASP:H	1.81	0.44
2:B:71:ALA:O	2:B:75:ILE:CG1	2.58	0.44
4:D:138:TYR:CD1	4:D:138:TYR:C	2.94	0.44
4:D:140:ASN:N	4:D:140:ASN:HD22	2.16	0.44
1:E:74:PHE:CD1	1:E:75:PRO:HD2	2.53	0.44
1:E:605:LYS:HD2	1:E:622:TYR:CB	2.47	0.44
1:E:608:LEU:HD23	1:E:608:LEU:N	2.32	0.44
2:F:205:PRO:HD3	9:F:303:F3S:S3	2.58	0.44
4:H:104:VAL:CG1	4:H:121:VAL:HG12	2.46	0.44
1:A:599:PHE:HA	1:A:602:HIS:CD2	2.52	0.44
2:B:217:ASP:O	2:B:219:ARG:N	2.50	0.44
2:F:139:MET:HB3	2:F:143:TYR:CE2	2.52	0.44
2:F:154:GLN:HE21	2:F:222:SER:HB2	1.83	0.44
2:F:196:TRP:CH2	3:G:59:HIS:HB2	2.53	0.44
2:F:251:LYS:HB2	2:F:253:LEU:HG	2.00	0.44
4:H:47:LYS:HB2	4:H:47:LYS:HE3	1.72	0.44
1:A:76:THR:CG2	1:A:182:HIS:NE2	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:TRP:CE3	1:A:158:ASN:HB3	2.52	0.44
1:A:486:ASP:OD2	1:A:529:ARG:HG2	2.17	0.44
1:A:538:ILE:O	1:A:539:TRP:O	2.35	0.44
3:C:132:THR:HG23	10:C:201:HEM:CBB	2.48	0.44
1:E:239:TYR:HB3	1:E:254:GLY:HA3	2.00	0.44
1:E:388:TYR:HE1	1:E:421:GLU:HG3	1.75	0.44
1:A:148:ILE:H	2:B:165:GLN:HE22	1.64	0.44
11:C:202:AT5:H142	4:D:107:TYR:CE2	2.52	0.44
1:E:46:ILE:HB	1:E:69:VAL:HG22	2.00	0.44
1:E:54:LEU:O	1:E:55:ARG:C	2.61	0.44
1:E:214:VAL:HG23	1:E:232:THR:HG21	1.99	0.44
1:E:570:ARG:HG3	1:E:581:ARG:CD	2.48	0.44
1:E:598:PRO:O	1:E:600:GLU:N	2.51	0.44
1:E:603:TRP:HZ3	1:E:622:TYR:CE2	2.36	0.44
2:B:141:LEU:HB2	3:C:45:TYR:CZ	2.53	0.44
3:C:143:MET:C	3:C:145:LYS:H	2.25	0.44
1:A:109:GLY:O	1:A:431:ASN:HB3	2.18	0.44
1:A:438:LEU:HG	6:A:702:FAD:C2	2.48	0.44
1:E:83:ALA:HB3	1:E:177:GLY:CA	2.45	0.44
1:E:437:SER:O	1:E:440:ASP:HB3	2.17	0.44
2:F:36:LYS:NZ	2:F:114:ASP:O	2.46	0.44
1:A:432:ARG:NH2	6:A:702:FAD:C2	2.81	0.43
3:C:45:TYR:O	3:C:49:GLN:HG2	2.18	0.43
3:G:43:TRP:O	3:G:44:ASP:C	2.61	0.43
1:A:126:ALA:HB2	1:A:439:LEU:HD11	2.01	0.43
2:B:102:ALA:HA	2:B:122:LYS:NZ	2.33	0.43
3:C:35:LYS:O	4:D:49:PHE:HE1	2.01	0.43
3:C:100:PHE:O	3:C:104:VAL:HG23	2.18	0.43
1:E:52:ALA:O	1:E:53:GLY:C	2.61	0.43
1:E:270:LEU:O	1:E:559:THR:HG23	2.18	0.43
2:F:34:ARG:HD3	2:F:34:ARG:O	2.18	0.43
3:G:168:LEU:O	3:G:172:VAL:HG12	2.18	0.43
10:G:201:HEM:CMB	10:G:201:HEM:CBB	2.93	0.43
1:A:56:ALA:O	1:A:57:ALA:C	2.61	0.43
2:B:145:GLN:O	2:B:148:SER:HB3	2.18	0.43
2:B:240:HIS:C	2:B:241:THR:HG22	2.43	0.43
3:C:43:TRP:CZ2	3:C:47:MET:HE3	2.53	0.43
1:E:131:THR:O	1:E:132:GLU:C	2.62	0.43
1:E:287:ILE:O	1:E:288:THR:O	2.37	0.43
2:F:154:GLN:HE21	2:F:222:SER:CB	2.30	0.43
1:A:98:ASP:C	1:A:100:LYS:N	2.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:71:VAL:HG12	3:C:72:SER:N	2.32	0.43
1:E:224:ILE:HG13	1:E:474:ILE:HD13	1.99	0.43
1:E:621:ASP:C	1:E:622:TYR:CD1	2.96	0.43
2:F:100:ASN:C	2:F:100:ASN:ND2	2.77	0.43
2:F:146:TYR:CE1	2:F:210:GLN:HG2	2.53	0.43
2:F:205:PRO:HA	2:F:259:ILE:HD11	2.01	0.43
1:A:155:GLY:HA3	1:A:433:LEU:HD11	1.99	0.43
1:A:242:ALA:HB2	1:A:552:LEU:HD22	2.00	0.43
1:A:359:ARG:C	1:A:360:LEU:HG	2.44	0.43
1:A:508:ARG:HB3	1:A:513:LEU:HD11	2.01	0.43
3:G:74:LEU:HD23	3:G:130:PHE:CE1	2.53	0.43
4:H:101:TRP:CH2	4:H:122:ARG:HG2	2.54	0.43
1:A:128:GLU:O	1:A:129:ALA:C	2.61	0.43
1:A:267:LEU:HB3	1:A:270:LEU:HD21	1.99	0.43
1:A:578:PHE:N	1:A:579:PRO:CD	2.82	0.43
4:D:73:ILE:N	4:D:74:PRO:CD	2.81	0.43
1:E:111:ASP:OD2	1:E:643:ARG:HD2	2.19	0.43
10:G:201:HEM:C1C	4:H:95:HIS:CD2	3.07	0.43
1:A:122:LEU:HG	1:A:439:LEU:CD1	2.48	0.43
1:A:267:LEU:HD12	1:A:558:GLN:OE1	2.18	0.43
1:A:428:HIS:HE1	1:A:436:ASN:HB3	1.83	0.43
1:A:433:LEU:HD12	1:A:434:GLY:H	1.84	0.43
1:A:577:ASP:C	1:A:579:PRO:HD3	2.42	0.43
2:B:141:LEU:O	2:B:142:PHE:C	2.62	0.43
1:E:117:ASN:OD1	1:E:397:TYR:HB3	2.18	0.43
1:E:337:VAL:HG12	1:E:343:HIS:O	2.19	0.43
4:H:77:TYR:HA	12:H:201:EPH:C1	2.48	0.43
2:B:239:CYS:C	2:B:241:THR:H	2.26	0.43
3:C:58:PRO:HB2	3:C:62:ILE:HG12	2.00	0.43
3:C:136:ILE:H	3:C:136:ILE:HG13	1.59	0.43
1:E:84:GLN:HB2	1:E:288:THR:HB	2.01	0.43
1:A:76:THR:O	1:A:76:THR:HG22	2.18	0.43
1:A:105:ASP:OD1	1:A:105:ASP:N	2.50	0.43
2:B:73:ILE:HG22	2:B:77:ASN:HD21	1.84	0.43
2:B:188:CYS:O	2:B:189:SER:C	2.61	0.43
2:B:268:LYS:HZ1	3:C:143:MET:HE2	1.84	0.43
1:E:496:MET:CE	1:E:552:LEU:HB3	2.44	0.43
1:E:623:ARG:HG3	1:E:624:PRO:HD2	2.01	0.43
1:A:291:SER:HB2	1:A:348:LEU:HD21	2.01	0.43
1:E:191:CYS:O	1:E:193:CYS:N	2.52	0.43
1:E:320:ARG:NH1	5:E:701:MLI:O6	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:544:THR:C	1:E:546:SER:H	2.26	0.43
2:F:276:LEU:HA	2:F:277:PRO:HD2	1.87	0.43
4:H:59:PHE:HE2	4:H:63:ARG:NH2	2.17	0.43
1:A:509:ARG:HB3	1:A:511:ASP:OD2	2.20	0.42
2:B:68:VAL:HG21	2:B:101:ILE:HD13	2.01	0.42
2:B:86:ARG:CD	2:B:136:VAL:HG13	2.49	0.42
2:B:185:CYS:HG	8:B:302:SF4:FE1	1.34	0.42
3:C:71:VAL:HG11	3:C:137:ARG:NH1	2.34	0.42
4:D:156:LEU:H	4:D:156:LEU:HG	1.67	0.42
1:E:300:ASN:HB3	1:E:306:PHE:CD2	2.54	0.42
1:A:78:SER:HB2	1:A:181:LEU:HD21	2.02	0.42
1:A:88:ASN:ND2	1:A:435:ALA:CB	2.80	0.42
3:C:126:PHE:HB3	3:C:127:PRO:HD3	2.01	0.42
1:A:72:LYS:HE2	6:A:702:FAD:C8A	2.49	0.42
1:A:134:GLU:OE2	2:B:219:ARG:NH1	2.45	0.42
1:A:205:LEU:HD22	1:A:214:VAL:O	2.19	0.42
1:A:453:LYS:O	1:A:453:LYS:HG3	2.18	0.42
2:B:86:ARG:HH11	2:B:137:PRO:HD2	1.83	0.42
2:B:262:ILE:HG22	2:B:266:LEU:HD22	2.01	0.42
4:D:87:CYS:HA	4:D:90:LEU:HB2	2.01	0.42
1:E:444:PHE:O	1:E:447:ALA:HB3	2.19	0.42
3:G:47:MET:HE2	3:G:47:MET:HA	2.01	0.42
3:G:156:ALA:O	3:G:160:LEU:HB2	2.19	0.42
1:A:370:PHE:HZ	2:B:110:ILE:HG22	1.84	0.42
2:B:97:CYS:O	2:B:98:ALA:C	2.62	0.42
2:B:208:LEU:HD13	2:B:259:ILE:CD1	2.44	0.42
3:C:126:PHE:HA	3:C:129:ALA:HB3	2.02	0.42
1:E:42:TYR:CD2	1:E:66:LYS:HG2	2.54	0.42
2:F:146:TYR:HE1	2:F:210:GLN:HG2	1.85	0.42
3:G:85:THR:O	3:G:89:GLY:N	2.52	0.42
3:G:97:PRO:O	3:G:98:LEU:C	2.63	0.42
4:H:69:MET:HE3	4:H:69:MET:HB3	1.72	0.42
3:C:66:GLN:O	3:C:70:MET:HB2	2.19	0.42
3:C:112:ILE:HG22	3:C:116:ILE:HD13	2.01	0.42
1:E:327:GLU:CD	1:E:344:ILE:HD11	2.44	0.42
1:E:331:ILE:CD1	1:E:344:ILE:HG23	2.49	0.42
1:E:388:TYR:CE2	1:E:432:ARG:HD2	2.55	0.42
3:G:85:THR:HA	3:G:88:ILE:HG13	2.00	0.42
1:A:219:LEU:HD23	1:A:219:LEU:HA	1.79	0.42
1:A:590:PRO:O	1:A:592:GLU:N	2.35	0.42
2:B:212:TYR:CZ	2:B:216:ILE:HG12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:HIS:HE1	2:F:184:LEU:HD22	1.77	0.42
2:F:141:LEU:O	2:F:145:GLN:HG3	2.19	0.42
3:G:104:VAL:HG13	4:H:156:LEU:HD23	2.02	0.42
1:A:34:GLN:NE2	1:A:35:TYR:H	2.18	0.42
1:A:93:SER:HB3	1:A:147:LYS:HB2	2.01	0.42
1:A:147:LYS:HA	2:B:165:GLN:HE22	1.83	0.42
1:A:585:TYR:CE1	1:A:596:LYS:HA	2.55	0.42
2:B:187:CYS:HB2	8:B:302:SF4:S3	2.60	0.42
2:B:189:SER:C	2:B:191:SER:H	2.28	0.42
1:E:45:VAL:O	1:E:232:THR:HA	2.20	0.42
1:E:56:ALA:HA	1:E:445:GLY:O	2.20	0.42
6:E:702:FAD:H1'1	6:E:702:FAD:H9	1.76	0.42
2:F:57:PHE:CG	2:F:75:ILE:HD12	2.52	0.42
2:F:146:TYR:HA	2:F:207:VAL:HG13	2.01	0.42
3:G:43:TRP:O	3:G:46:LEU:N	2.52	0.42
3:G:170:VAL:O	3:G:174:PRO:HD2	2.18	0.42
1:A:110:SER:HA	1:A:428:HIS:O	2.19	0.42
2:B:261:GLU:O	2:B:265:LEU:HD12	2.20	0.42
1:E:146:GLY:HA3	2:F:167:TYR:HE1	1.84	0.42
1:A:234:VAL:HG12	1:A:236:THR:HG23	2.02	0.42
1:A:580:LYS:HB3	1:A:582:GLU:OE1	2.20	0.42
4:D:109:ARG:NH2	4:D:109:ARG:CG	2.72	0.42
10:G:201:HEM:NC	4:H:95:HIS:HD2	1.99	0.42
1:A:219:LEU:HD21	1:A:544:THR:HG21	2.01	0.42
1:E:309:ARG:NH2	1:E:310:TYR:CE2	2.88	0.42
1:E:410:ASP:OD2	1:E:410:ASP:N	2.52	0.42
2:F:135:LEU:HD23	2:F:135:LEU:HA	1.80	0.42
2:B:224:ALA:HB3	2:B:225:GLU:OE2	2.19	0.41
2:B:230:MET:HE1	2:B:262:ILE:HD13	2.02	0.41
3:C:73:GLY:O	3:C:76:ARG:HB2	2.19	0.41
1:E:72:LYS:HE2	6:E:702:FAD:N7A	2.34	0.41
1:E:236:THR:OG1	1:E:256:GLY:HA3	2.20	0.41
1:E:251:MET:HE2	2:F:88:SER:HB2	2.02	0.41
1:E:401:VAL:HG21	1:E:416:LEU:HG	2.01	0.41
2:F:209:MET:HE3	2:F:258:ALA:CB	2.47	0.41
1:A:536:SER:HB2	2:B:46:GLU:OE1	2.20	0.41
3:C:173:TYR:CD1	3:C:173:TYR:C	2.98	0.41
1:E:79:HIS:NE2	6:E:702:FAD:C8	2.75	0.41
1:E:83:ALA:HA	6:E:702:FAD:C5X	2.50	0.41
1:E:207:ASP:OD1	1:E:208:LYS:HG3	2.20	0.41
1:E:389:ASN:O	1:E:390:MET:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:71:ALA:O	2:F:75:ILE:HG12	2.20	0.41
4:H:80:HIS:HA	4:H:147:THR:HG21	2.01	0.41
1:A:72:LYS:HE2	6:A:702:FAD:N7A	2.35	0.41
1:A:133:LEU:HD23	1:A:133:LEU:HA	1.89	0.41
1:A:231:ARG:HH11	1:A:456:LEU:HD23	1.85	0.41
2:B:42:ARG:HD2	2:B:42:ARG:HA	1.85	0.41
2:B:131:VAL:CG2	3:C:55:PRO:HG2	2.50	0.41
2:B:242:ILE:HG12	3:C:72:SER:OG	2.20	0.41
1:E:88:ASN:ND2	1:E:156:GLN:HE22	2.17	0.41
1:E:237:GLY:HA2	1:E:421:GLU:HB3	2.02	0.41
1:E:286:LEU:HD12	1:E:286:LEU:C	2.45	0.41
1:E:448:CYS:O	1:E:452:ILE:HG13	2.19	0.41
1:E:466:PRO:O	1:E:469:ALA:HB2	2.20	0.41
2:F:39:GLU:HB2	2:F:122:LYS:HB2	2.01	0.41
2:F:97:CYS:HB2	2:F:108:ALA:HB3	2.03	0.41
1:A:268:GLU:CB	1:A:608:LEU:HD23	2.46	0.41
1:A:346:LEU:HB2	1:A:382:VAL:HG21	2.02	0.41
1:A:375:VAL:HG12	1:A:380:ILE:HD11	2.02	0.41
3:C:52:LEU:C	3:C:54:ARG:H	2.29	0.41
4:D:140:ASN:HD22	4:D:145:GLY:HA2	1.86	0.41
1:E:238:GLY:HA3	1:E:389:ASN:ND2	2.34	0.41
1:E:325:ARG:O	1:E:328:THR:N	2.52	0.41
1:A:99:TRP:CZ2	1:A:100:LYS:HE3	2.56	0.41
1:A:420:GLY:O	1:A:421:GLU:C	2.63	0.41
1:E:231:ARG:HH11	1:E:456:LEU:HD23	1.85	0.41
1:E:276:HIS:NE2	1:E:286:LEU:HD11	2.35	0.41
1:A:111:ASP:CG	1:A:643:ARG:HD3	2.45	0.41
1:A:262:ARG:HH12	1:A:551:ASN:ND2	2.18	0.41
1:A:277:PRO:HD3	1:A:320:ARG:HB3	2.01	0.41
1:A:433:LEU:HD12	1:A:433:LEU:HA	1.82	0.41
2:F:158:LYS:HE3	2:F:158:LYS:HB2	1.42	0.41
1:A:499:THR:O	1:A:500:MET:C	2.63	0.41
1:A:509:ARG:HD2	1:A:511:ASP:OD2	2.21	0.41
2:B:69:LEU:HD12	2:B:109:CYS:HB3	2.02	0.41
2:B:142:PHE:CE1	2:B:206:ALA:HB3	2.56	0.41
1:E:73:MET:HE3	6:E:702:FAD:H3B	2.03	0.41
2:F:242:ILE:CG1	11:G:202:AT5:HM33	2.51	0.41
4:H:117:LEU:O	4:H:121:VAL:HG23	2.21	0.41
1:A:43:ASP:HB2	1:A:66:LYS:O	2.21	0.41
1:A:300:ASN:HB2	1:A:301:SER:H	1.72	0.41
1:A:393:ILE:O	1:A:395:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:ASN:OD1	2:B:105:ASN:ND2	2.53	0.41
2:B:196:TRP:CE3	3:C:59:HIS:HB2	2.55	0.41
3:C:137:ARG:NH2	3:C:141:PHE:HZ	2.19	0.41
3:C:166:ILE:O	3:C:170:VAL:HB	2.21	0.41
10:C:201:HEM:HMB1	10:C:201:HEM:CBB	2.37	0.41
1:E:142:ARG:HG2	2:F:168:GLN:O	2.20	0.41
1:E:244:PHE:CD1	1:E:498:LYS:HE3	2.56	0.41
1:E:480:VAL:HG21	1:E:550:GLN:NE2	2.35	0.41
3:G:137:ARG:O	3:G:140:GLY:N	2.53	0.41
1:A:172:VAL:O	1:A:174:ASP:N	2.54	0.41
1:A:499:THR:O	1:A:502:LYS:N	2.53	0.41
1:A:585:TYR:CZ	1:A:596:LYS:HD3	2.56	0.41
1:E:117:ASN:O	1:E:120:HIS:HB3	2.20	0.41
1:E:122:LEU:CD1	1:E:440:ASP:HA	2.51	0.41
1:E:159:ASN:O	1:E:162:LYS:HG2	2.20	0.41
1:E:214:VAL:HG12	1:E:215:ILE:H	1.85	0.41
1:E:249:ALA:C	1:E:251:MET:N	2.79	0.41
1:E:433:LEU:HD12	1:E:433:LEU:HA	1.92	0.41
2:F:155:LYS:HA	2:F:221:ASP:HB2	2.02	0.41
2:F:242:ILE:HG23	3:G:69:TRP:HA	2.03	0.41
3:G:47:MET:HE2	3:G:47:MET:N	2.36	0.41
3:G:49:GLN:OE1	3:G:54:ARG:NH1	2.54	0.41
1:A:93:SER:HB3	1:A:147:LYS:HB3	2.02	0.41
1:A:98:ASP:O	1:A:100:LYS:N	2.54	0.41
1:A:99:TRP:HH2	1:A:120:HIS:HE1	1.69	0.41
2:B:174:GLU:O	2:B:177:ASP:HB2	2.21	0.41
2:B:189:SER:HA	2:B:205:PRO:HG2	2.03	0.41
3:C:154:ARG:O	3:C:155:GLY:C	2.64	0.41
1:E:492:LEU:HD21	1:E:527:LEU:HD12	2.02	0.41
1:E:513:LEU:O	1:E:517:VAL:HG23	2.21	0.41
1:E:627:ASP:O	1:E:637:TRP:HB2	2.21	0.41
1:A:230:LYS:CD	1:A:462:ILE:HA	2.49	0.40
2:B:69:LEU:HB2	2:B:109:CYS:HA	2.03	0.40
2:B:197:TRP:O	4:D:109:ARG:NH2	2.54	0.40
1:E:219:LEU:HD23	1:E:219:LEU:HA	1.78	0.40
1:E:562:ALA:HB1	1:E:607:THR:HG21	2.02	0.40
4:H:124:GLY:O	4:H:128:PHE:N	2.55	0.40
4:H:127:ILE:HD13	4:H:127:ILE:HA	1.80	0.40
3:C:83:ALA:HB1	4:D:96:VAL:HG11	2.04	0.40
1:E:48:GLY:HA2	6:E:702:FAD:H1B	2.02	0.40
1:E:77:ARG:NH1	2:F:94:CYS:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:169:ALA:O	3:G:170:VAL:C	2.63	0.40
1:A:121:TYR:HE1	1:A:447:ALA:HB2	1.87	0.40
1:A:271:GLU:HB2	1:A:563:ALA:HB2	2.03	0.40
1:A:434:GLY:O	1:A:435:ALA:CB	2.70	0.40
1:A:532:THR:OG1	1:A:535:ARG:NH2	2.51	0.40
1:E:337:VAL:HG11	1:E:345:TYR:CD1	2.56	0.40
1:E:361:PRO:HG2	1:E:362:GLY:N	2.35	0.40
1:E:544:THR:O	1:E:545:GLU:C	2.63	0.40
1:E:561:VAL:CG2	1:E:620:LEU:HD11	2.51	0.40
1:E:612:ASP:HA	1:E:613:PRO:HD2	1.76	0.40
2:F:39:GLU:HB3	2:F:54:LEU:HD22	2.03	0.40
2:F:188:CYS:SG	2:F:189:SER:N	2.94	0.40
2:F:197:TRP:HA	4:H:109:ARG:HH22	1.85	0.40
3:G:71:VAL:HG11	3:G:137:ARG:HH12	1.86	0.40
1:A:249:ALA:C	1:A:251:MET:H	2.28	0.40
1:A:266:ALA:HB2	1:A:610:LYS:CG	2.52	0.40
1:A:457:LYS:C	1:A:459:ASP:H	2.29	0.40
1:E:393:ILE:HA	1:E:394:PRO:HD3	1.97	0.40
1:E:397:TYR:CE1	1:E:398:LYS:HG3	2.56	0.40
1:E:623:ARG:NH2	1:E:626:ILE:HD11	2.36	0.40
1:A:95:ASN:HA	1:A:96:PRO:HD2	1.90	0.40
1:A:279:GLY:HA3	1:A:385:THR:OG1	2.21	0.40
1:A:496:MET:HE1	1:A:552:LEU:HB3	2.03	0.40
3:C:104:VAL:HG21	4:D:152:MET:HE3	2.03	0.40
3:C:105:GLU:C	3:C:107:ILE:N	2.80	0.40
3:G:75:HIS:CE1	3:G:131:HIS:CE1	3.09	0.40
4:H:54:SER:C	4:H:56:GLY:N	2.79	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	611/645 (95%)	493 (81%)	92 (15%)	26 (4%)	2	16
1	E	611/645 (95%)	499 (82%)	82 (13%)	30 (5%)	1	14
2	B	247/282 (88%)	204 (83%)	34 (14%)	9 (4%)	2	19
2	F	247/282 (88%)	192 (78%)	42 (17%)	13 (5%)	1	12
3	C	151/188 (80%)	110 (73%)	34 (22%)	7 (5%)	2	15
3	G	151/188 (80%)	118 (78%)	25 (17%)	8 (5%)	1	12
4	D	127/156 (81%)	96 (76%)	27 (21%)	4 (3%)	3	22
4	H	127/156 (81%)	87 (68%)	32 (25%)	8 (6%)	1	10
All	All	2272/2542 (89%)	1799 (79%)	368 (16%)	105 (5%)	2	15

All (105) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	THR
1	A	614	ARG
2	B	89	CYS
3	C	97	PRO
4	D	49	PHE
1	E	127	VAL
1	E	269	ASP
1	E	288	THR
1	E	339	PRO
1	E	485	GLY
1	E	590	PRO
1	E	591	ILE
1	E	599	PHE
2	F	89	CYS
3	G	98	LEU
3	G	111	GLY
4	H	29	SER
4	H	115	ASP
1	A	305	ARG
1	A	391	GLY
1	A	407	GLU
1	A	426	SER
1	A	458	PRO
1	A	460	GLU
1	A	469	ALA
1	A	485	GLY
1	A	539	TRP

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Mol	Chain	Res	Type
2	B	49	GLY
2	B	134	ASP
2	B	224	ALA
2	B	277	PRO
3	C	155	GLY
1	E	51	GLY
1	E	326	ALA
1	E	391	GLY
1	E	460	GLU
1	E	621	ASP
2	F	132	ILE
2	F	161	LEU
2	F	199	ALA
3	G	185	PRO
4	H	51	PRO
1	A	259	LEU
1	A	483	ALA
1	A	524	SER
1	A	538	ILE
1	A	592	GLU
2	B	205	PRO
2	B	218	SER
3	C	37	PRO
3	C	90	GLY
3	C	106	PHE
4	D	47	LYS
4	D	85	ASP
1	E	173	ALA
1	E	260	ALA
1	E	527	LEU
2	F	204	GLY
2	F	205	PRO
2	F	268	LYS
2	F	279	PRO
3	G	74	LEU
3	G	183	THR
1	A	99	TRP
1	A	173	ALA
1	A	590	PRO
2	B	280	ALA
3	C	98	LEU
1	E	53	GLY

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Mol	Chain	Res	Type
1	E	128	GLU
1	E	179	SER
1	E	192	HIS
1	E	364	SER
1	E	463	PRO
1	E	604	ARG
1	E	629	THR
2	F	277	PRO
4	H	55	HIS
1	A	96	PRO
1	A	194	THR
1	A	252	ASN
1	A	308	GLU
1	A	591	ILE
2	B	140	ASN
3	C	150	PRO
1	E	250	HIS
1	E	305	ARG
2	F	48	PRO
2	F	52	PRO
3	G	59	HIS
3	G	97	PRO
4	H	77	TYR
1	A	381	PRO
1	E	429	GLY
1	E	458	PRO
2	F	88	SER
4	H	154	TRP
4	D	50	LYS
1	E	462	ILE
2	F	273	PRO
3	G	150	PRO
1	A	505	GLY
1	E	381	PRO
4	H	36	ALA
4	H	144	VAL

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	498/526 (95%)	401 (80%)	97 (20%)	1 7
1	E	498/526 (95%)	412 (83%)	86 (17%)	2 10
2	B	219/242 (90%)	165 (75%)	54 (25%)	1 3
2	F	219/242 (90%)	173 (79%)	46 (21%)	1 5
3	C	127/158 (80%)	93 (73%)	34 (27%)	0 2
3	G	127/158 (80%)	104 (82%)	23 (18%)	2 9
4	D	96/119 (81%)	68 (71%)	28 (29%)	0 2
4	H	96/119 (81%)	71 (74%)	25 (26%)	0 2
All	All	1880/2090 (90%)	1487 (79%)	393 (21%)	1 5

All (393) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	37	VAL
1	A	39	ASP
1	A	47	ILE
1	A	60	LEU
1	A	71	THR
1	A	93	SER
1	A	105	ASP
1	A	108	LYS
1	A	113	LEU
1	A	117	ASN
1	A	131	THR
1	A	142	ARG
1	A	152	SER
1	A	175	ARG
1	A	179	SER
1	A	203	ASP
1	A	205	LEU
1	A	211	CYS
1	A	214	VAL
1	A	230	LYS
1	A	257	THR
1	A	261	THR
1	A	265	ILE

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Mol	Chain	Res	Type
1	A	270	LEU
1	A	280	ILE
1	A	283	VAL
1	A	285	CYS
1	A	298	LEU
1	A	299	VAL
1	A	304	GLU
1	A	313	LYS
1	A	320	ARG
1	A	321	ASP
1	A	322	VAL
1	A	335	ARG
1	A	344	ILE
1	A	351	LEU
1	A	354	GLU
1	A	356	LEU
1	A	359	ARG
1	A	368	LYS
1	A	377	LYS
1	A	382	VAL
1	A	383	ILE
1	A	385	THR
1	A	390	MET
1	A	401	VAL
1	A	405	THR
1	A	412	ILE
1	A	417	TYR
1	A	422	CYS
1	A	425	HIS
1	A	426	SER
1	A	427	VAL
1	A	439	LEU
1	A	440	ASP
1	A	443	VAL
1	A	449	SER
1	A	450	ILE
1	A	452	ILE
1	A	453	LYS
1	A	454	GLU
1	A	455	GLU
1	A	456	LEU
1	A	461	LYS

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Mol	Chain	Res	Type
1	A	462	ILE
1	A	474	ILE
1	A	487	VAL
1	A	492	LEU
1	A	496	MET
1	A	502	LYS
1	A	518	LYS
1	A	525	LYS
1	A	526	GLU
1	A	528	LYS
1	A	531	LYS
1	A	535	ARG
1	A	549	LEU
1	A	552	LEU
1	A	560	ILE
1	A	561	VAL
1	A	564	GLU
1	A	584	GLU
1	A	591	ILE
1	A	596	LYS
1	A	597	ARG
1	A	601	LYS
1	A	612	ASP
1	A	618	ILE
1	A	628	LYS
1	A	629	THR
1	A	630	LEU
1	A	637	TRP
1	A	638	ILE
1	A	642	ILE
1	A	644	SER
2	B	34	ARG
2	B	39	GLU
2	B	40	ILE
2	B	42	ARG
2	B	46	GLU
2	B	47	GLU
2	B	54	LEU
2	B	59	VAL
2	B	63	LYS
2	B	64	CYS
2	B	69	LEU

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Mol	Chain	Res	Type
2	B	73	ILE
2	B	75	ILE
2	B	83	LEU
2	B	87	ARG
2	B	90	ARG
2	B	93	ILE
2	B	106	THR
2	B	115	GLN
2	B	117	THR
2	B	119	LYS
2	B	120	THR
2	B	122	LYS
2	B	129	MET
2	B	139	MET
2	B	148	SER
2	B	149	ILE
2	B	154	GLN
2	B	156	LYS
2	B	157	THR
2	B	159	ILE
2	B	164	LYS
2	B	169	SER
2	B	170	ILE
2	B	171	LYS
2	B	172	GLU
2	B	173	GLN
2	B	174	GLU
2	B	179	LEU
2	B	194	SER
2	B	209	MET
2	B	215	ILE
2	B	216	ILE
2	B	227	LEU
2	B	238	LYS
2	B	244	ASN
2	B	246	THR
2	B	247	LYS
2	B	253	LEU
2	B	266	LEU
2	B	268	LYS
2	B	269	MET
2	B	272	LYS

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Mol	Chain	Res	Type
2	B	281	ASN
3	C	34	GLU
3	C	50	ARG
3	C	53	LYS
3	C	59	HIS
3	C	61	THR
3	C	67	MET
3	C	71	VAL
3	C	72	SER
3	C	77	VAL
3	C	85	THR
3	C	87	LEU
3	C	94	SER
3	C	95	VAL
3	C	96	LEU
3	C	98	LEU
3	C	99	ASP
3	C	102	THR
3	C	110	LEU
3	C	112	ILE
3	C	115	VAL
3	C	118	ASP
3	C	127	PRO
3	C	133	LEU
3	C	136	ILE
3	C	149	ILE
3	C	158	LEU
3	C	160	LEU
3	C	162	LEU
3	C	165	LEU
3	C	168	LEU
3	C	170	VAL
3	C	173	TYR
3	C	175	ARG
3	C	177	GLU
4	D	33	THR
4	D	43	ILE
4	D	46	GLU
4	D	47	LYS
4	D	49	PHE
4	D	50	LYS
4	D	53	HIS

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Mol	Chain	Res	Type
4	D	63	ARG
4	D	69	MET
4	D	79	ILE
4	D	82	ARG
4	D	83	GLU
4	D	86	LEU
4	D	90	LEU
4	D	92	LEU
4	D	93	THR
4	D	104	VAL
4	D	109	ARG
4	D	117	LEU
4	D	121	VAL
4	D	123	VAL
4	D	136	LEU
4	D	140	ASN
4	D	143	ASP
4	D	144	VAL
4	D	152	MET
4	D	153	VAL
4	D	156	LEU
1	E	34	GLN
1	E	44	VAL
1	E	45	VAL
1	E	47	ILE
1	E	62	GLU
1	E	70	VAL
1	E	76	THR
1	E	80	THR
1	E	81	THR
1	E	99	TRP
1	E	117	ASN
1	E	122	LEU
1	E	127	VAL
1	E	131	THR
1	E	153	PHE
1	E	160	TYR
1	E	162	LYS
1	E	165	VAL
1	E	170	CYS
1	E	194	THR
1	E	197	ILE

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Mol	Chain	Res	Type
1	E	198	GLU
1	E	203	ASP
1	E	205	LEU
1	E	210	ARG
1	E	223	THR
1	E	226	ARG
1	E	228	ARG
1	E	230	LYS
1	E	231	ARG
1	E	232	THR
1	E	257	THR
1	E	265	ILE
1	E	269	ASP
1	E	270	LEU
1	E	274	GLN
1	E	288	THR
1	E	301	SER
1	E	313	LYS
1	E	320	ARG
1	E	322	VAL
1	E	324	SER
1	E	328	THR
1	E	337	VAL
1	E	344	ILE
1	E	351	LEU
1	E	355	GLN
1	E	359	ARG
1	E	376	THR
1	E	377	LYS
1	E	385	THR
1	E	405	THR
1	E	406	LYS
1	E	410	ASP
1	E	411	LYS
1	E	425	HIS
1	E	426	SER
1	E	436	ASN
1	E	453	LYS
1	E	454	GLU
1	E	461	LYS
1	E	474	ILE
1	E	487	VAL

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Mol	Chain	Res	Type
1	E	491	GLU
1	E	494	LEU
1	E	496	MET
1	E	498	LYS
1	E	511	ASP
1	E	520	MET
1	E	523	LEU
1	E	525	LYS
1	E	526	GLU
1	E	533	THR
1	E	535	ARG
1	E	537	LEU
1	E	547	LEU
1	E	561	VAL
1	E	564	GLU
1	E	585	TYR
1	E	595	THR
1	E	608	LEU
1	E	609	THR
1	E	628	LYS
1	E	634	GLU
1	E	637	TRP
1	E	642	ILE
2	F	34	ARG
2	F	37	THR
2	F	46	GLU
2	F	51	LYS
2	F	63	LYS
2	F	66	THR
2	F	69	LEU
2	F	73	ILE
2	F	90	ARG
2	F	93	ILE
2	F	100	ASN
2	F	115	GLN
2	F	117	THR
2	F	122	LYS
2	F	128	HIS
2	F	129	MET
2	F	131	VAL
2	F	139	MET
2	F	156	LYS

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Mol	Chain	Res	Type
2	F	158	LYS
2	F	159	ILE
2	F	161	LEU
2	F	164	LYS
2	F	169	SER
2	F	170	ILE
2	F	171	LYS
2	F	172	GLU
2	F	176	LEU
2	F	184	LEU
2	F	194	SER
2	F	201	LYS
2	F	209	MET
2	F	215	ILE
2	F	227	LEU
2	F	230	MET
2	F	241	THR
2	F	244	ASN
2	F	247	LYS
2	F	248	THR
2	F	261	GLU
2	F	265	LEU
2	F	266	LEU
2	F	268	LYS
2	F	270	LYS
2	F	276	LEU
2	F	278	THR
3	G	40	VAL
3	G	50	ARG
3	G	53	LYS
3	G	66	GLN
3	G	67	MET
3	G	95	VAL
3	G	98	LEU
3	G	99	ASP
3	G	102	THR
3	G	105	GLU
3	G	110	LEU
3	G	112	ILE
3	G	118	ASP
3	G	119	THR
3	G	133	LEU

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Mol	Chain	Res	Type
3	G	139	ILE
3	G	149	ILE
3	G	151	SER
3	G	159	VAL
3	G	162	LEU
3	G	179	HIS
3	G	181	LYS
3	G	186	THR
4	H	46	GLU
4	H	47	LYS
4	H	53	HIS
4	H	61	ILE
4	H	64	TYR
4	H	70	VAL
4	H	72	LEU
4	H	73	ILE
4	H	79	ILE
4	H	82	ARG
4	H	83	GLU
4	H	84	MET
4	H	86	LEU
4	H	88	LEU
4	H	94	LEU
4	H	109	ARG
4	H	112	VAL
4	H	117	LEU
4	H	122	ARG
4	H	123	VAL
4	H	131	CYS
4	H	136	LEU
4	H	143	ASP
4	H	153	VAL
4	H	156	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	117	ASN
1	A	120	HIS
1	A	150	GLN
1	A	178	HIS

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Mol	Chain	Res	Type
1	A	252	ASN
1	A	428	HIS
1	A	431	ASN
1	A	436	ASN
1	A	451	ASN
1	A	484	ASN
1	A	550	GLN
1	A	551	ASN
1	A	555	ASN
1	A	558	GLN
1	A	565	ASN
1	A	611	GLN
2	B	44	ASN
2	B	55	GLN
2	B	77	ASN
2	B	100	ASN
2	B	105	ASN
2	B	112	ASN
2	B	115	GLN
2	B	128	HIS
2	B	145	GLN
2	B	165	GLN
3	C	59	HIS
4	D	140	ASN
1	E	88	ASN
1	E	95	ASN
1	E	117	ASN
1	E	120	HIS
1	E	156	GLN
1	E	159	ASN
1	E	178	HIS
1	E	182	HIS
1	E	347	GLN
1	E	349	HIS
1	E	355	GLN
1	E	358	GLN
1	E	389	ASN
1	E	436	ASN
1	E	451	ASN
1	E	484	ASN
1	E	550	GLN
1	E	551	ASN

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Mol	Chain	Res	Type
1	E	602	HIS
1	E	606	HIS
1	E	611	GLN
2	F	55	GLN
2	F	100	ASN
2	F	105	ASN
2	F	115	GLN
2	F	116	ASN
2	F	154	GLN
2	F	165	GLN
2	F	210	GLN
2	F	244	ASN
4	H	140	ASN

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)

16 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	$\#\|Z\| > 2$
11	AT5	G	202	-	20,23,23	1.97	5 (25%)	21,32,32	1.41	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	EPH	D	201	-	43,43,48	1.93	8 (18%)	46,48,53	2.45	8 (17%)
8	SF4	F	302	2	0,12,12	-	-	-		
11	AT5	C	202	-	20,23,23	2.10	7 (35%)	21,32,32	2.48	3 (14%)
7	FES	F	301	2	0,4,4	-	-	-		
12	EPH	H	201	-	43,43,48	2.08	11 (25%)	46,48,53	2.76	9 (19%)
10	HEM	G	201	3,4	50,50,50	2.14	13 (26%)	67,82,82	1.23	6 (8%)
6	FAD	A	702	-	58,58,58	1.25	8 (13%)	85,89,89	1.76	22 (25%)
7	FES	B	301	2	0,4,4	-	-	-		
5	MLI	E	701	-	6,6,6	4.38	2 (33%)	7,7,7	2.16	4 (57%)
10	HEM	C	201	3,4	50,50,50	1.93	10 (20%)	67,82,82	1.37	8 (11%)
5	MLI	A	701	-	6,6,6	4.71	2 (33%)	7,7,7	1.70	2 (28%)
9	F3S	B	303	2	0,9,9	-	-	-		
6	FAD	E	702	-	58,58,58	1.18	5 (8%)	85,89,89	2.01	26 (30%)
8	SF4	B	302	2	0,12,12	-	-	-		
9	F3S	F	303	2	0,9,9	-	-	-		

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
11	AT5	G	202	-	-	16/20/22/22	0/1/1/1
12	EPH	D	201	-	-	19/47/47/52	-
12	EPH	H	201	-	-	21/47/47/52	-
11	AT5	C	202	-	-	12/20/22/22	0/1/1/1
7	FES	F	301	2	-	-	0/1/1/1
8	SF4	F	302	2	-	-	0/6/5/5
10	HEM	G	201	3,4	-	8/14/54/54	-
6	FAD	A	702	-	-	16/34/50/50	0/6/6/6
7	FES	B	301	2	-	-	0/1/1/1
10	HEM	C	201	3,4	-	7/14/54/54	-
5	MLI	E	701	-	-	2/4/4/4	-
5	MLI	A	701	-	-	2/4/4/4	-
9	F3S	B	303	2	-	-	0/3/3/3
6	FAD	E	702	-	-	11/34/50/50	0/6/6/6
8	SF4	B	302	2	-	-	0/6/5/5
9	F3S	F	303	2	-	-	0/3/3/3

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	701	MLI	C1-C2	-11.04	1.34	1.51
5	E	701	MLI	C1-C2	-10.27	1.35	1.51
10	C	201	HEM	C3D-C2D	7.95	1.53	1.36
10	G	201	HEM	C3D-C2D	7.88	1.53	1.36
12	H	201	EPH	C29-C28	7.19	1.72	1.31
12	D	201	EPH	C29-C28	7.07	1.71	1.31
11	C	202	AT5	O4-C5	6.80	1.36	1.23
10	G	201	HEM	FE-NA	6.22	2.15	1.95
11	G	202	AT5	O4-C5	5.99	1.34	1.23
10	G	201	HEM	FE-ND	5.19	2.10	1.94
6	A	702	FAD	C4X-N5	4.48	1.40	1.30
10	C	201	HEM	FE-ND	4.32	2.08	1.94
10	C	201	HEM	FE-NC	4.24	2.09	1.95
12	D	201	EPH	C13-C12	4.01	1.54	1.31
12	H	201	EPH	C13-C12	3.94	1.54	1.31
12	H	201	EPH	C25-C24	3.93	1.54	1.31
6	E	702	FAD	C4X-N5	3.92	1.39	1.30
10	G	201	HEM	FE-NB	3.87	2.06	1.94
12	D	201	EPH	C25-C24	3.86	1.53	1.31
12	D	201	EPH	C18-C4	-3.75	1.39	1.50
12	H	201	EPH	C18-C4	-3.57	1.40	1.50
12	H	201	EPH	C15-C16	3.47	1.54	1.29
12	D	201	EPH	C15-C16	3.43	1.54	1.29
10	C	201	HEM	CAB-C3B	3.24	1.56	1.47
10	G	201	HEM	CAB-C3B	3.17	1.55	1.47
6	A	702	FAD	C9A-N10	-3.12	1.35	1.41
12	D	201	EPH	C27-C28	-3.03	1.33	1.50
12	D	201	EPH	P1-O7	3.03	1.61	1.50
11	G	202	AT5	C6-C7	3.02	1.56	1.47
12	H	201	EPH	C26-C25	3.00	1.66	1.50
12	D	201	EPH	C26-C25	2.93	1.66	1.50
6	E	702	FAD	C10-N1	2.90	1.39	1.33
6	A	702	FAD	C2A-N1A	2.87	1.39	1.33
11	C	202	AT5	C11-C12	-2.84	1.49	1.54
11	G	202	AT5	C11-C12	-2.83	1.49	1.54
12	H	201	EPH	C27-C28	-2.79	1.34	1.50
10	C	201	HEM	FE-NB	2.78	2.03	1.94
12	H	201	EPH	P1-O7	2.76	1.60	1.50
12	H	201	EPH	C5-C3	2.71	1.58	1.50
6	E	702	FAD	C2A-N3A	2.65	1.38	1.33
6	A	702	FAD	C2A-N3A	2.64	1.38	1.33
10	C	201	HEM	CAD-C3D	2.56	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	702	FAD	C2A-N1A	2.56	1.38	1.33
10	G	201	HEM	CAC-C3C	2.55	1.54	1.47
11	C	202	AT5	C5-N4	-2.55	1.34	1.38
11	G	202	AT5	C5-N4	-2.54	1.34	1.38
10	C	201	HEM	CAC-C3C	2.52	1.54	1.47
10	G	201	HEM	CMB-C2B	2.51	1.55	1.50
10	C	201	HEM	C2A-C3A	-2.50	1.32	1.38
10	G	201	HEM	CAD-C3D	2.46	1.57	1.51
12	H	201	EPH	O2-C4	2.38	1.40	1.33
11	C	202	AT5	C6-C7	2.30	1.54	1.47
6	A	702	FAD	C8A-N7A	2.27	1.36	1.31
11	C	202	AT5	O3-CM3	-2.25	1.40	1.45
10	G	201	HEM	CMD-C2D	2.23	1.55	1.50
10	G	201	HEM	C3C-C2C	-2.23	1.32	1.37
11	C	202	AT5	C6-C5	-2.23	1.39	1.44
6	A	702	FAD	C5A-N7A	-2.19	1.35	1.39
10	G	201	HEM	C2A-C3A	-2.17	1.33	1.38
10	G	201	HEM	CMC-C2C	2.14	1.55	1.50
10	C	201	HEM	C3C-C2C	-2.13	1.32	1.37
6	E	702	FAD	C8A-N7A	2.12	1.35	1.31
5	E	701	MLI	C1-C3	-2.09	1.47	1.51
12	H	201	EPH	C37-C2	2.08	1.57	1.50
10	C	201	HEM	CMB-C2B	2.07	1.55	1.50
6	A	702	FAD	P-O3P	2.05	1.61	1.59
5	A	701	MLI	C1-C3	-2.03	1.47	1.51
10	G	201	HEM	CMA-C3A	2.02	1.54	1.50
6	A	702	FAD	C10-N1	2.02	1.37	1.33
11	G	202	AT5	C3-N4	-2.01	1.34	1.37
11	C	202	AT5	C3-N4	-2.01	1.34	1.37

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	H	201	EPH	C27-C26-C25	13.42	146.45	112.73
12	D	201	EPH	C27-C26-C25	12.48	144.08	112.73
11	C	202	AT5	C8-C11-C12	-8.19	100.42	115.09
12	H	201	EPH	C2-O1-C3	7.26	135.17	117.80
6	E	702	FAD	N3A-C2A-N1A	-6.16	119.26	128.58
12	H	201	EPH	C15-C14-C13	5.96	141.35	112.02
12	D	201	EPH	C15-C14-C13	5.83	140.76	112.02
6	A	702	FAD	N3A-C2A-N1A	-5.39	120.43	128.58
10	C	201	HEM	C4D-ND-C1D	4.99	111.12	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	702	FAD	N9A-C8A-N7A	-4.89	107.00	113.94
11	C	202	AT5	C11-C12-C13	-4.82	101.92	110.11
6	E	702	FAD	C8M-C8-C9	-4.77	111.17	119.57
11	C	202	AT5	C14-C13-CL12	4.57	118.38	108.64
12	D	201	EPH	C2-O1-C3	4.49	128.53	117.80
6	E	702	FAD	C5X-C9A-N10	4.41	121.96	117.97
10	G	201	HEM	C4D-ND-C1D	4.21	110.19	105.21
6	A	702	FAD	C9-C9A-N10	-4.11	116.32	121.85
6	A	702	FAD	C5A-C4A-N3A	-4.05	121.14	126.72
6	E	702	FAD	C5A-N7A-C8A	3.76	109.36	103.45
6	E	702	FAD	C5A-C4A-N3A	-3.73	121.58	126.72
6	E	702	FAD	C8M-C8-C7	3.64	128.19	120.76
6	E	702	FAD	C2A-N3A-C4A	3.62	120.68	111.83
6	E	702	FAD	O4-C4-C4X	-3.52	117.25	126.53
6	A	702	FAD	C4-C4X-N5	3.44	122.96	118.21
6	A	702	FAD	N9A-C8A-N7A	-3.42	109.08	113.94
6	E	702	FAD	C4A-N9A-C8A	3.39	109.30	105.74
6	A	702	FAD	C5A-N7A-C8A	3.36	108.73	103.45
11	G	202	AT5	C11-C12-C13	-3.33	104.44	110.11
12	D	201	EPH	C14-C15-C16	3.19	150.58	123.74
6	A	702	FAD	C4A-C5A-N7A	-3.19	106.93	110.58
10	C	201	HEM	CAA-C2A-C1A	3.17	131.13	124.94
6	A	702	FAD	C4'-C3'-C2'	-3.15	108.33	113.57
6	E	702	FAD	C4-N3-C2	-3.14	120.06	125.64
5	E	701	MLI	C3-C1-C2	3.14	124.04	112.95
10	G	201	HEM	CAD-C3D-C4D	3.12	130.13	124.70
6	A	702	FAD	C2A-N3A-C4A	3.11	119.42	111.83
12	H	201	EPH	C14-C15-C16	3.06	149.48	123.74
10	C	201	HEM	CAD-C3D-C4D	3.04	129.99	124.70
6	A	702	FAD	C5X-C9A-N10	3.04	120.72	117.97
6	E	702	FAD	C9-C9A-N10	-3.03	117.78	121.85
6	E	702	FAD	C4X-C4-N3	3.01	120.92	113.25
6	A	702	FAD	C9A-C5X-N5	-2.91	119.37	122.45
12	H	201	EPH	O2-C1-C2	2.82	116.53	108.40
6	A	702	FAD	C4X-C4-N3	2.81	120.39	113.25
6	E	702	FAD	C4A-C5A-N7A	-2.79	107.39	110.58
6	A	702	FAD	O4B-C1B-N9A	2.71	113.30	108.09
11	G	202	AT5	C14-C13-CL12	2.70	114.41	108.64
6	A	702	FAD	C8M-C8-C9	-2.69	114.83	119.57
6	E	702	FAD	O2-C2-N1	-2.65	117.40	121.80
6	E	702	FAD	O4B-C1B-N9A	2.64	113.17	108.09
6	E	702	FAD	O2'-C2'-C3'	-2.62	103.11	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	701	MLI	C3-C1-C2	2.60	122.13	112.95
6	A	702	FAD	C5A-C4A-N9A	2.59	108.63	105.81
5	E	701	MLI	O7-C2-C1	2.57	122.48	114.51
10	C	201	HEM	CAA-CBA-CGA	-2.57	106.86	113.67
10	C	201	HEM	CAA-C2A-C3A	-2.53	121.39	127.07
6	E	702	FAD	N3A-C4A-N9A	2.53	131.47	127.17
6	E	702	FAD	C4X-C10-N10	2.53	120.10	116.48
10	G	201	HEM	C4C-C3C-C2C	2.52	109.00	106.81
5	E	701	MLI	O9-C3-C1	2.50	122.27	114.51
6	A	702	FAD	C4-N3-C2	-2.48	121.23	125.64
6	E	702	FAD	C4A-N9A-C1B	-2.47	120.86	126.63
6	E	702	FAD	O2-C2-N3	2.46	123.30	118.58
6	A	702	FAD	C4X-C10-N10	2.40	119.92	116.48
6	A	702	FAD	C10-C4X-N5	-2.40	119.91	124.81
12	D	201	EPH	C19-C18-C4	2.38	122.41	113.69
10	C	201	HEM	O2D-CGD-CBD	2.37	121.50	114.00
6	E	702	FAD	C9A-C5X-N5	-2.36	119.95	122.45
10	C	201	HEM	CBD-CAD-C3D	2.36	119.06	112.53
12	H	201	EPH	C1-O2-C4	2.26	125.37	117.12
6	E	702	FAD	C1'-C2'-C3'	2.25	115.75	109.66
12	D	201	EPH	C37-C2-C1	-2.23	106.58	111.78
5	E	701	MLI	O6-C2-C1	-2.22	115.79	122.11
12	H	201	EPH	O2-C4-C18	2.21	118.58	111.83
10	G	201	HEM	CMD-C2D-C1D	2.21	128.49	125.03
12	D	201	EPH	O8-C38-C39	2.21	117.25	109.17
6	A	702	FAD	O2P-P-O3P	2.21	113.24	107.27
12	H	201	EPH	O1-C2-C37	2.19	116.20	108.34
6	A	702	FAD	C6-C5X-N5	2.18	122.06	118.44
10	G	201	HEM	C4D-C3D-C2D	-2.15	103.76	106.89
6	A	702	FAD	C8M-C8-C7	2.14	125.13	120.76
5	A	701	MLI	O7-C2-C1	2.12	121.09	114.51
11	G	202	AT5	C6-C5-N4	2.12	120.95	115.10
12	H	201	EPH	O5-P1-O7	-2.12	100.54	108.94
12	D	201	EPH	C30-C29-C28	-2.12	113.69	126.42
6	E	702	FAD	O3P-P-O1P	-2.11	104.35	110.70
10	G	201	HEM	CBD-CAD-C3D	2.11	118.36	112.53
6	E	702	FAD	C7M-C7-C8	2.06	124.96	120.76
11	G	202	AT5	C17-C12-C11	-2.04	107.59	110.68
10	C	201	HEM	CMD-C2D-C1D	2.03	128.21	125.03
6	A	702	FAD	O3B-C3B-C4B	-2.03	105.26	111.08
6	E	702	FAD	C3B-C2B-C1B	2.01	105.26	101.46

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	702	FAD	N10-C1'-C2'-O2'
6	A	702	FAD	N10-C1'-C2'-C3'
6	A	702	FAD	C1'-C2'-C3'-O3'
6	A	702	FAD	C1'-C2'-C3'-C4'
6	A	702	FAD	O4'-C4'-C5'-O5'
6	E	702	FAD	C5B-O5B-PA-O1A
6	E	702	FAD	N10-C1'-C2'-O2'
6	E	702	FAD	N10-C1'-C2'-C3'
10	C	201	HEM	C2C-C3C-CAC-CBC
10	C	201	HEM	C4C-C3C-CAC-CBC
10	C	201	HEM	C2D-C3D-CAD-CBD
10	G	201	HEM	C2C-C3C-CAC-CBC
10	G	201	HEM	C4C-C3C-CAC-CBC
10	G	201	HEM	C2D-C3D-CAD-CBD
10	G	201	HEM	C4D-C3D-CAD-CBD
11	C	202	AT5	C5-C6-C7-O5
11	C	202	AT5	C1-C6-C7-O5
11	C	202	AT5	C5-C6-C7-C8
11	C	202	AT5	C1-C6-C7-C8
11	C	202	AT5	C12-C11-C8-C7
11	C	202	AT5	C12-C11-C8-C10
11	C	202	AT5	C11-C12-C13-CL12
11	C	202	AT5	C11-C12-C13-C14
11	C	202	AT5	C17-C12-C13-CL12
11	C	202	AT5	C17-C12-C13-C14
11	G	202	AT5	C5-C6-C7-O5
11	G	202	AT5	C1-C6-C7-O5
11	G	202	AT5	C5-C6-C7-C8
11	G	202	AT5	C1-C6-C7-C8
11	G	202	AT5	C11-C12-C13-CL12
11	G	202	AT5	C17-C12-C13-CL12
12	D	201	EPH	C27-C28-C29-C30
12	D	201	EPH	C37-O5-P1-O7
12	D	201	EPH	C38-O8-P1-O5
12	D	201	EPH	C38-O8-P1-O7
12	H	201	EPH	C38-O8-P1-O7
12	H	201	EPH	O8-C38-C39-N1
10	C	201	HEM	C4D-C3D-CAD-CBD
12	H	201	EPH	C5-C3-O1-C2
10	C	201	HEM	C1A-C2A-CAA-CBA
10	C	201	HEM	C2A-CAA-CBA-CGA
10	C	201	HEM	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	H	201	EPH	O3-C3-O1-C2
12	D	201	EPH	C18-C4-O2-C1
6	A	702	FAD	O2'-C2'-C3'-O3'
12	D	201	EPH	O4-C4-O2-C1
6	A	702	FAD	O2'-C2'-C3'-C4'
6	E	702	FAD	O3'-C3'-C4'-C5'
6	A	702	FAD	C2'-C3'-C4'-C5'
12	H	201	EPH	C3-C5-C6-C7
12	H	201	EPH	C23-C24-C25-C26
12	H	201	EPH	C11-C12-C13-C14
12	H	201	EPH	C20-C21-C22-C23
11	G	202	AT5	CL12-C13-C14-CL16
6	A	702	FAD	O3'-C3'-C4'-C5'
12	D	201	EPH	C20-C21-C22-C23
12	D	201	EPH	C7-C8-C9-C10
6	A	702	FAD	C2'-C3'-C4'-O4'
12	H	201	EPH	C28-C29-C30-C31
12	D	201	EPH	C18-C19-C20-C21
6	E	702	FAD	C2'-C3'-C4'-O4'
12	H	201	EPH	C4-C18-C19-C20
6	A	702	FAD	C3'-C4'-C5'-O5'
12	H	201	EPH	C6-C7-C8-C9
12	H	201	EPH	C21-C22-C23-C24
12	D	201	EPH	C23-C24-C25-C26
6	E	702	FAD	O3'-C3'-C4'-O4'
12	H	201	EPH	C1-C2-C37-O5
5	A	701	MLI	C2-C1-C3-O8
5	E	701	MLI	C2-C1-C3-O8
12	H	201	EPH	C25-C26-C27-C28
11	G	202	AT5	O5-C7-C8-C10
12	H	201	EPH	O2-C1-C2-O1
12	D	201	EPH	C12-C13-C14-C15
12	H	201	EPH	C12-C13-C14-C15
6	A	702	FAD	PA-O3P-P-O5'
6	E	702	FAD	PA-O3P-P-O5'
6	E	702	FAD	C2'-C3'-C4'-C5'
12	H	201	EPH	C37-C2-O1-C3
12	H	201	EPH	O1-C2-C37-O5
12	D	201	EPH	C11-C12-C13-C14
11	G	202	AT5	C12-C11-C8-C10
5	A	701	MLI	C2-C1-C3-O9
11	G	202	AT5	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
12	D	201	EPH	C26-C27-C28-C29
12	H	201	EPH	C26-C27-C28-C29
11	G	202	AT5	C12-C13-C14-CL16
6	A	702	FAD	C5B-O5B-PA-O1A
6	A	702	FAD	C5B-O5B-PA-O2A
6	A	702	FAD	C5B-O5B-PA-O3P
12	D	201	EPH	C38-O8-P1-O6
10	G	201	HEM	C3D-CAD-CBD-CGD
11	C	202	AT5	C8-C11-C12-C13
6	E	702	FAD	P-O3P-PA-O2A
5	E	701	MLI	C2-C1-C3-O9
11	G	202	AT5	C12-C11-C8-C7
12	H	201	EPH	C22-C23-C24-C25
6	A	702	FAD	O3'-C3'-C4'-O4'
11	G	202	AT5	C17-C12-C13-C14
12	H	201	EPH	C18-C19-C20-C21
11	G	202	AT5	C6-C7-C8-C11
11	C	202	AT5	C8-C11-C12-C17
11	G	202	AT5	C8-C11-C12-C13
10	G	201	HEM	C2A-CAA-CBA-CGA
10	G	201	HEM	CAD-CBD-CGD-O2D
12	D	201	EPH	C28-C29-C30-C31
12	D	201	EPH	C22-C23-C24-C25
12	D	201	EPH	C24-C25-C26-C27
10	G	201	HEM	CAD-CBD-CGD-O1D
6	E	702	FAD	P-O3P-PA-O1A
6	E	702	FAD	O4B-C4B-C5B-O5B
11	G	202	AT5	C8-C11-C12-C17
12	D	201	EPH	C14-C15-C16-C17
12	D	201	EPH	C6-C7-C8-C9

There are no ring outliers.

13 monomers are involved in 101 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	G	202	AT5	11	0
12	D	201	EPH	4	0
11	C	202	AT5	12	0
7	F	301	FES	1	0
12	H	201	EPH	2	0
10	G	201	HEM	15	0
6	A	702	FAD	12	0

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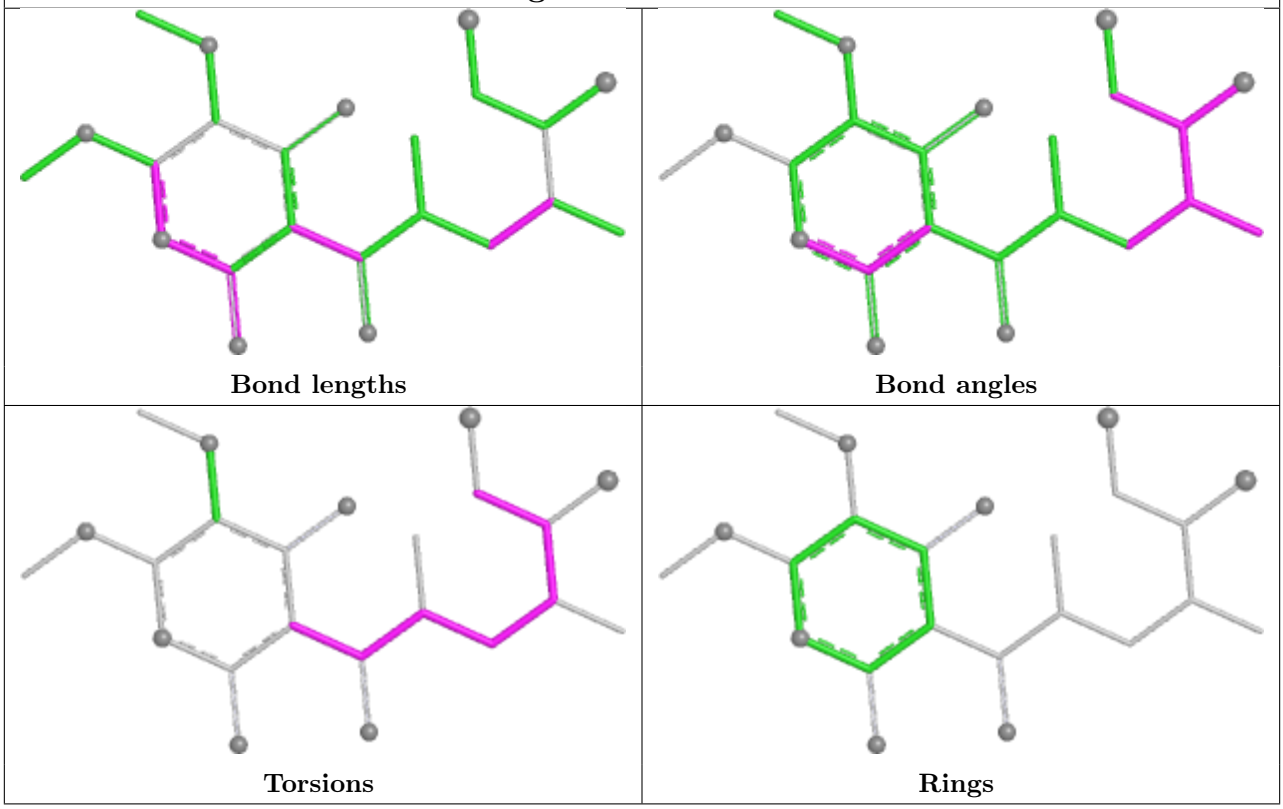
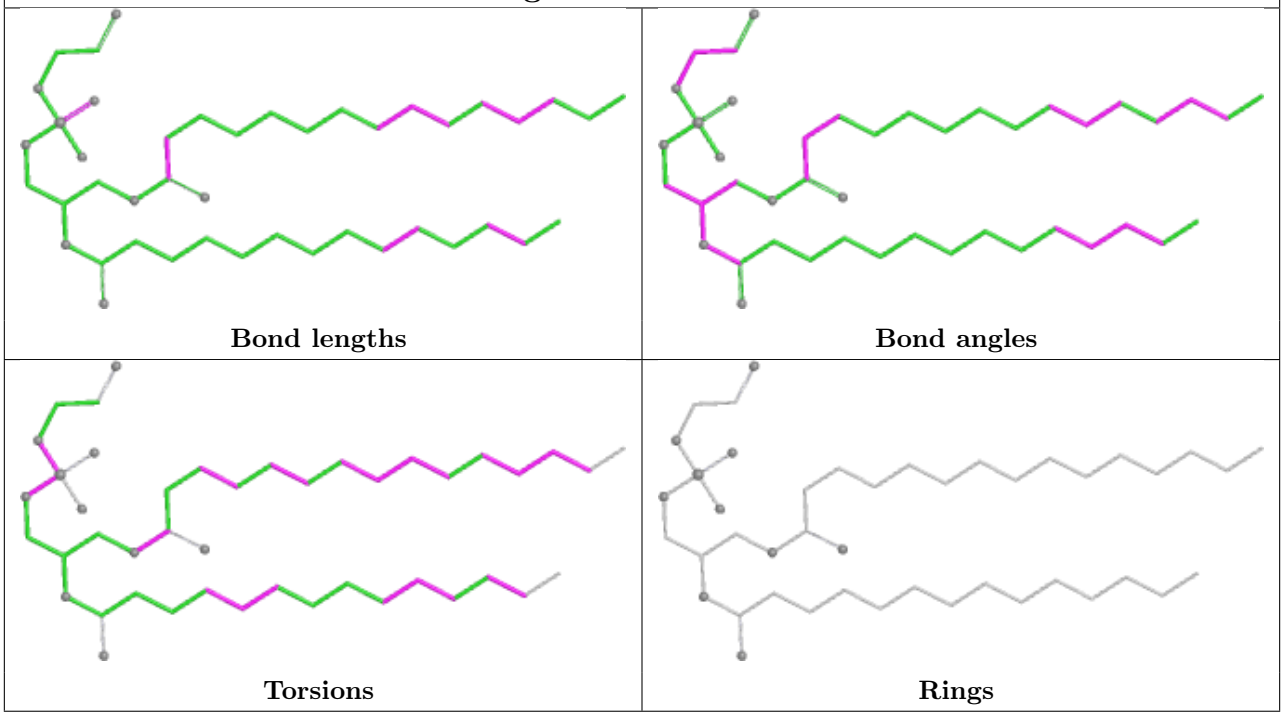
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	701	MLI	4	0
10	C	201	HEM	14	0
5	A	701	MLI	3	0
6	E	702	FAD	18	0
8	B	302	SF4	5	0
9	F	303	F3S	2	0

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 then 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.

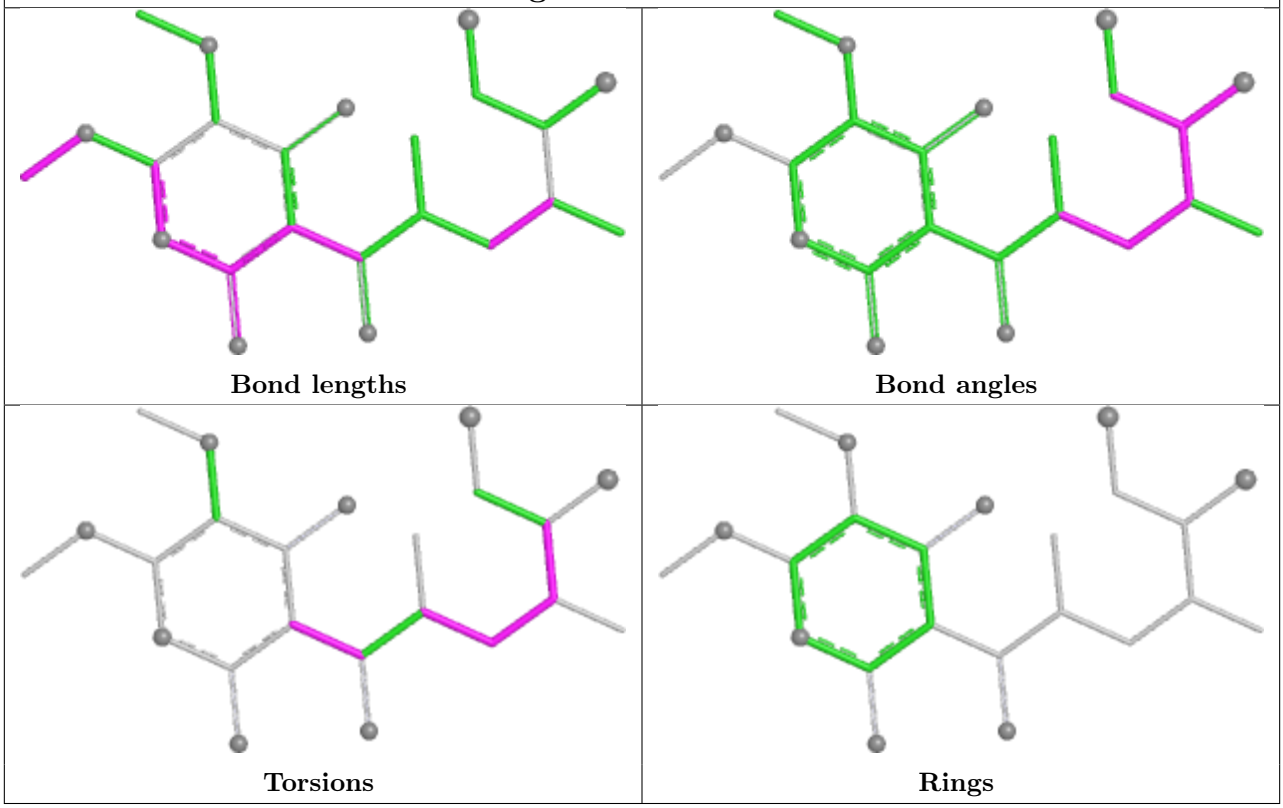
Ligand AT5 G 202

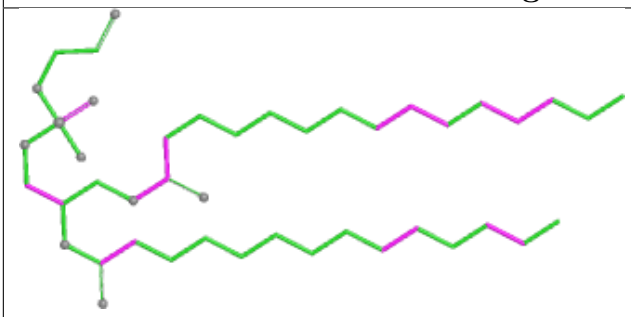
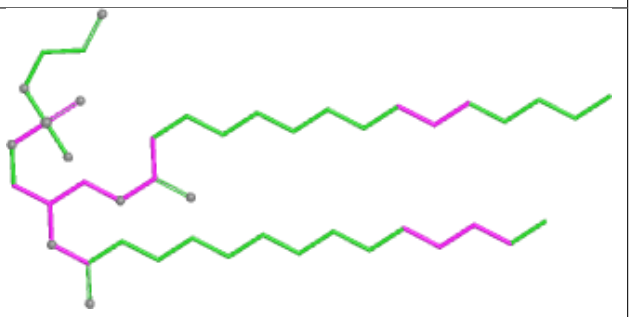
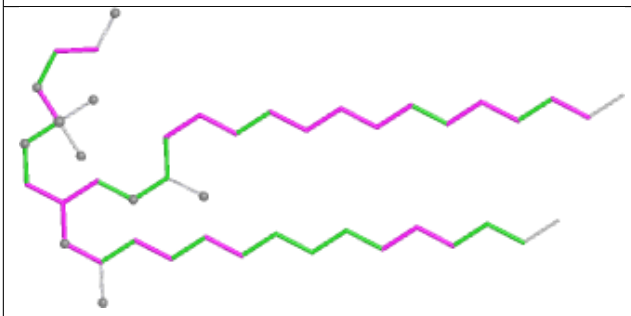
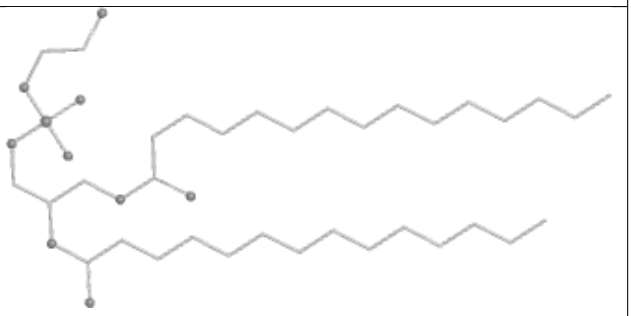


Ligand EPH D 201

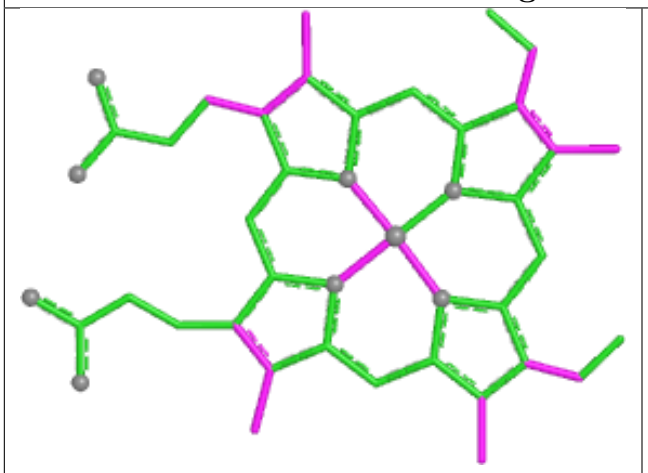


Ligand AT5 C 202

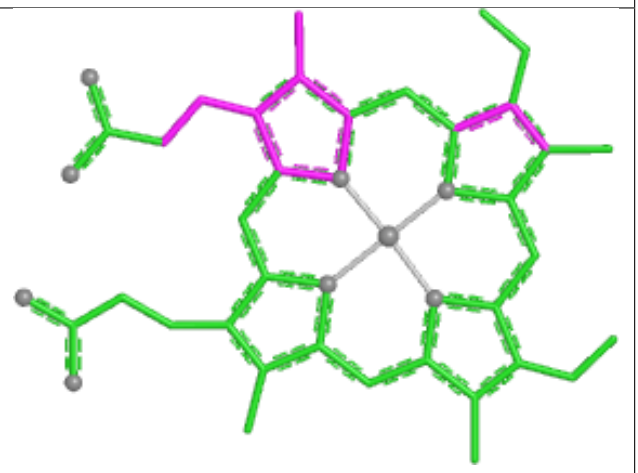


Ligand EPH H 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

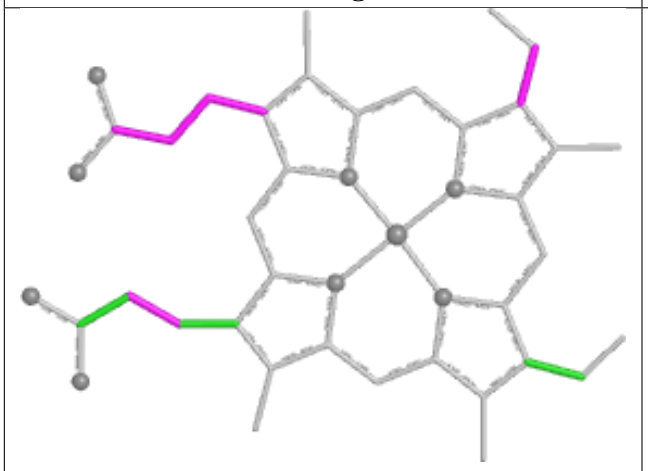
Ligand HEM G 201



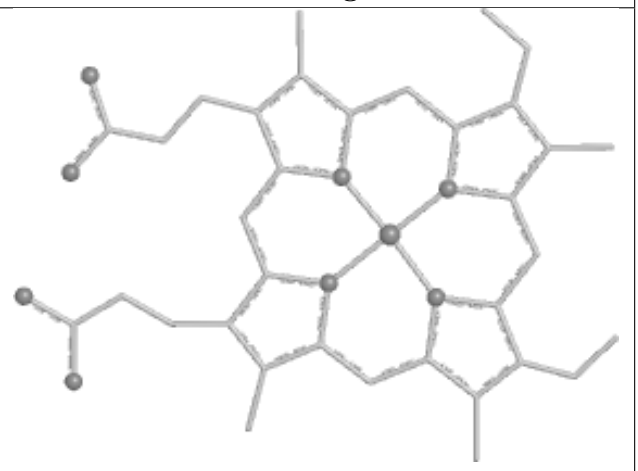
Bond lengths



Bond angles

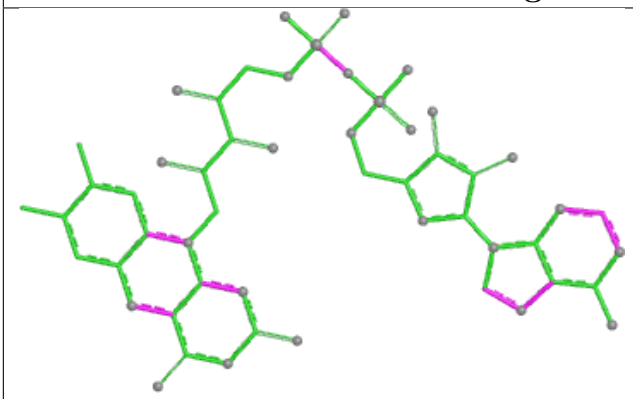


Torsions

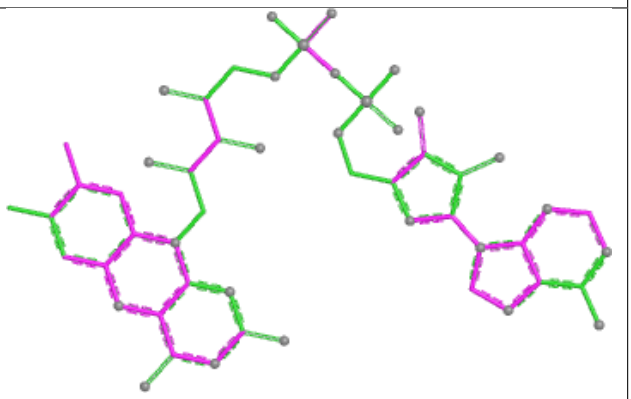


Rings

Ligand FAD A 702



Bond lengths



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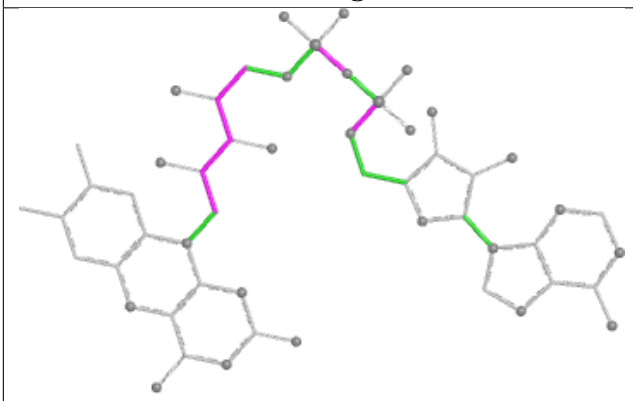

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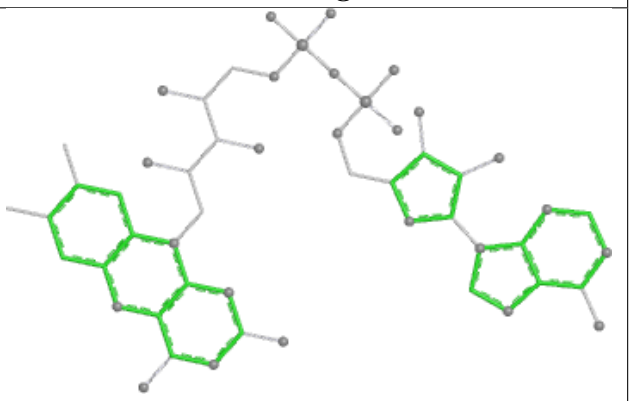
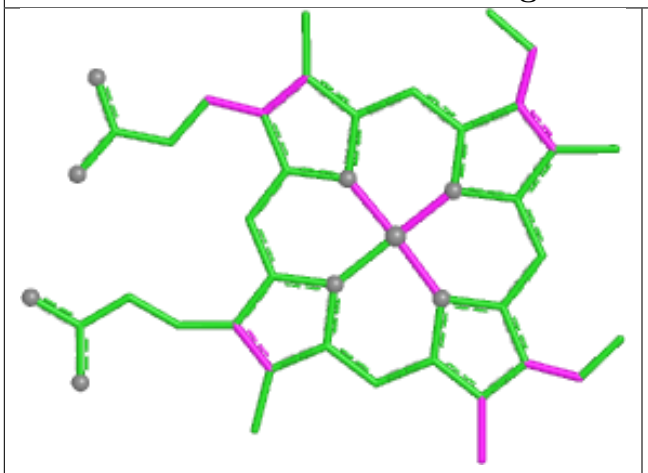


Rings

Ligand HEM C 201



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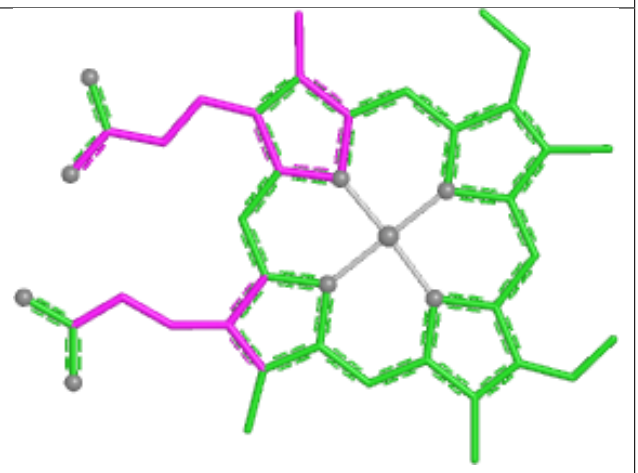
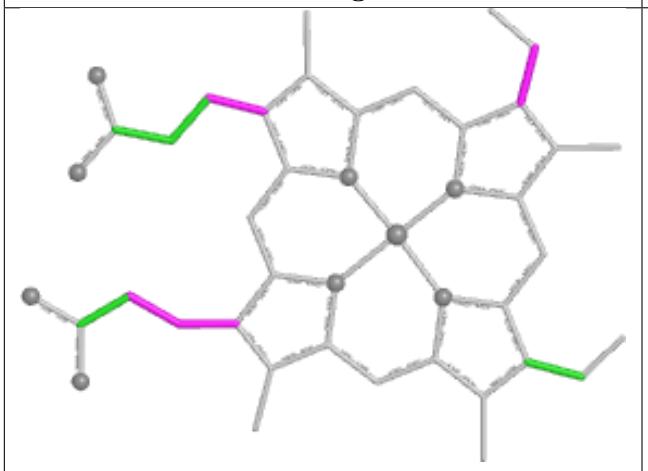


Bond angles



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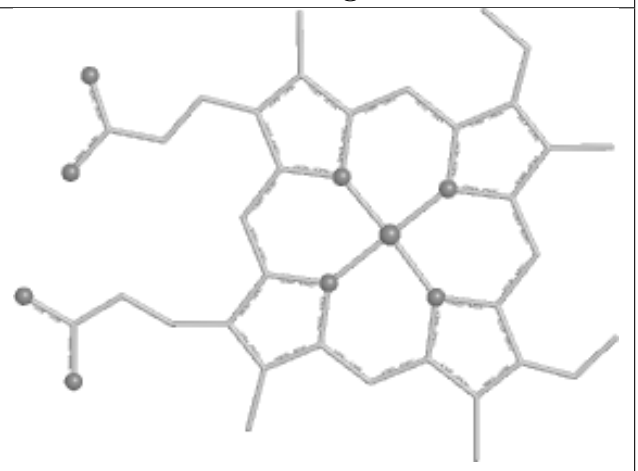
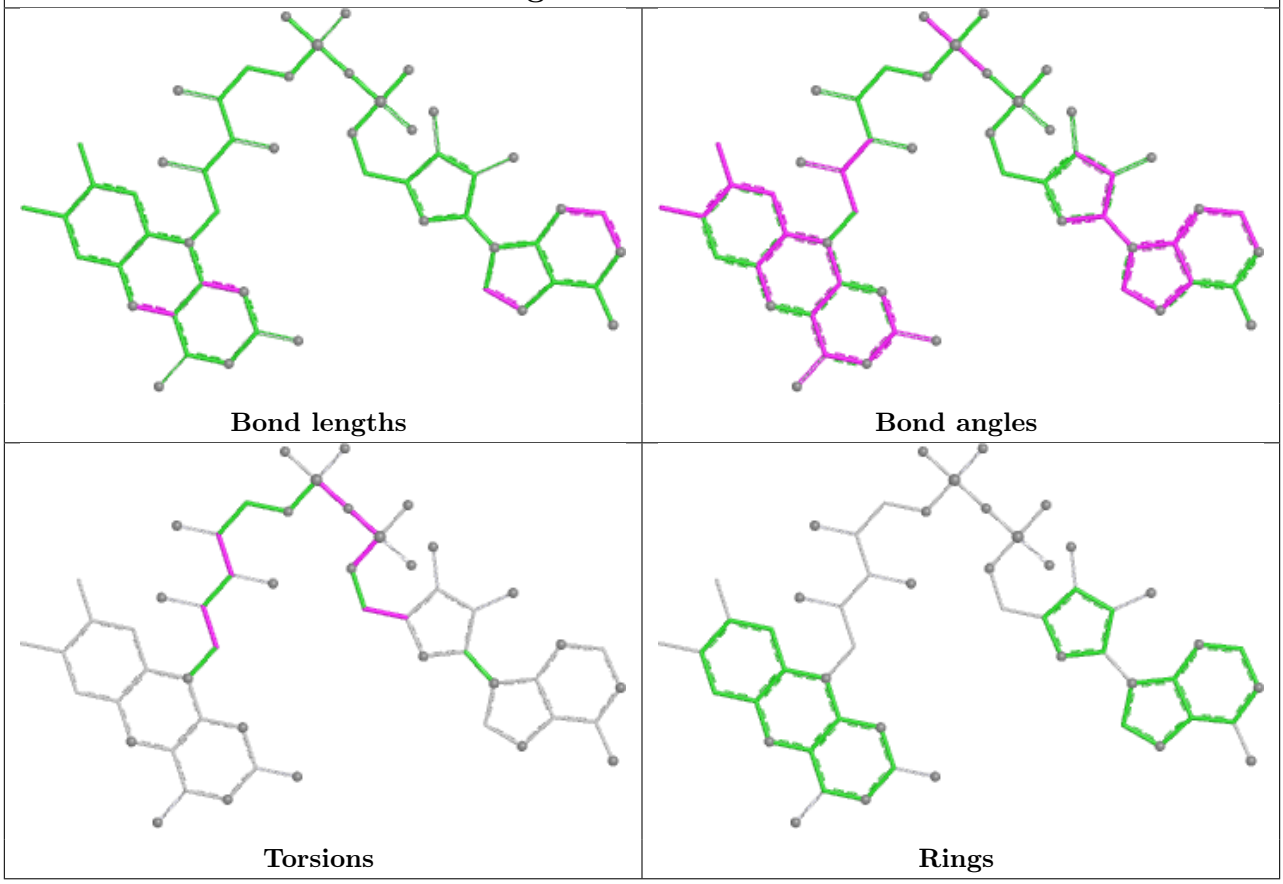


Rings

Ligand FAD E 702



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	613/645 (95%)	-0.33	4 (0%)	84	67	84, 111, 132, 145	0
1	E	613/645 (95%)	-0.40	4 (0%)	84	67	78, 105, 126, 141	0
2	B	249/282 (88%)	-0.35	1 (0%)	88	76	78, 99, 125, 146	0
2	F	249/282 (88%)	-0.49	2 (0%)	82	64	71, 92, 114, 130	0
3	C	153/188 (81%)	-0.26	2 (1%)	75	55	89, 107, 148, 165	0
3	G	153/188 (81%)	-0.29	2 (1%)	75	55	88, 101, 172, 199	0
4	D	129/156 (82%)	-0.35	0	100	100	92, 107, 131, 142	0
4	H	129/156 (82%)	-0.15	4 (3%)	51	34	90, 109, 145, 151	0
All	All	2288/2542 (90%)	-0.35	19 (0%)	82	64	71, 106, 134, 199	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	572	ALA	4.2
2	B	247	LYS	3.9
1	E	425	HIS	3.0
3	C	67	MET	2.6
1	A	282	GLY	2.6
4	H	52	LEU	2.5
4	H	29	SER	2.5
1	E	448	CYS	2.4
4	H	45	ALA	2.4
3	C	182	ALA	2.3
1	E	444	PHE	2.3
3	G	35	LYS	2.3
1	A	237	GLY	2.2
1	A	166	ALA	2.2
2	F	110	ILE	2.1
4	H	49	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	264	MET	2.0
1	E	445	GLY	2.0
3	G	184	LEU	2.0

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)

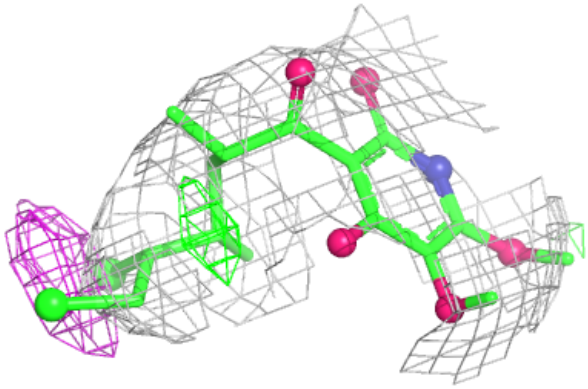
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

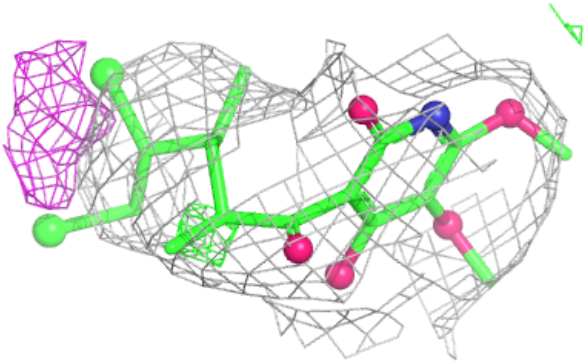
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	AT5	C	202	23/23	0.83	0.16	110,115,144,151	0
11	AT5	G	202	23/23	0.84	0.14	115,121,134,148	0
5	MLI	A	701	7/7	0.91	0.07	99,101,101,102	0
12	EPH	H	201	44/49	0.92	0.17	101,138,160,161	0
10	HEM	G	201	43/43	0.94	0.13	111,117,126,129	0
5	MLI	E	701	7/7	0.94	0.12	95,96,96,96	0
12	EPH	D	201	44/49	0.95	0.17	114,133,158,158	0
6	FAD	E	702	53/53	0.96	0.07	63,76,88,90	0
6	FAD	A	702	53/53	0.96	0.07	69,90,95,96	0
10	HEM	C	201	43/43	0.97	0.10	105,108,121,127	0
7	FES	F	301	4/4	0.99	0.02	82,85,88,89	0
9	F3S	B	303	7/7	0.99	0.05	89,90,92,93	0
7	FES	B	301	4/4	1.00	0.02	78,78,80,82	0
9	F3S	F	303	7/7	1.00	0.03	79,82,83,83	0
8	SF4	B	302	8/8	1.00	0.02	67,72,75,75	0
8	SF4	F	302	8/8	1.00	0.02	57,65,68,68	0

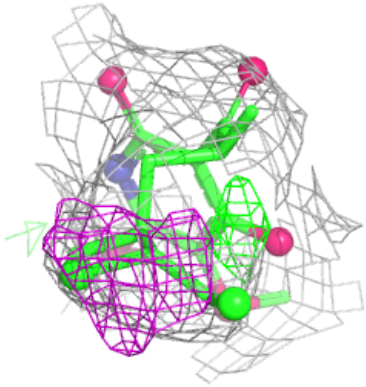
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AT5 C 202:

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







Electron density around AT5 G 202:

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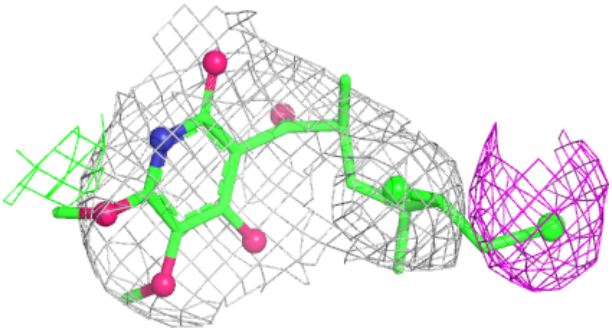
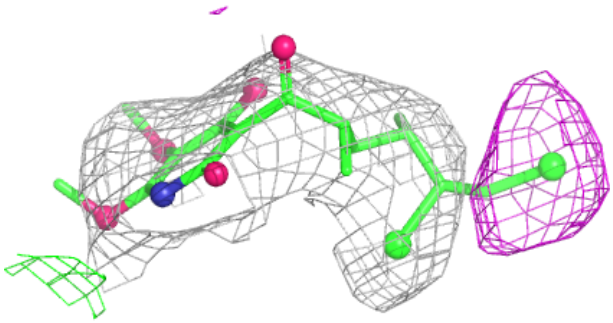
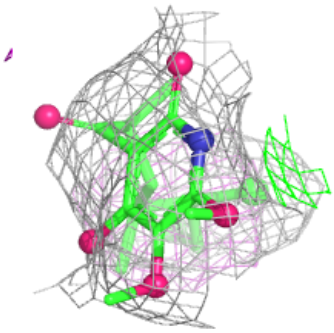
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around EPH H 201:

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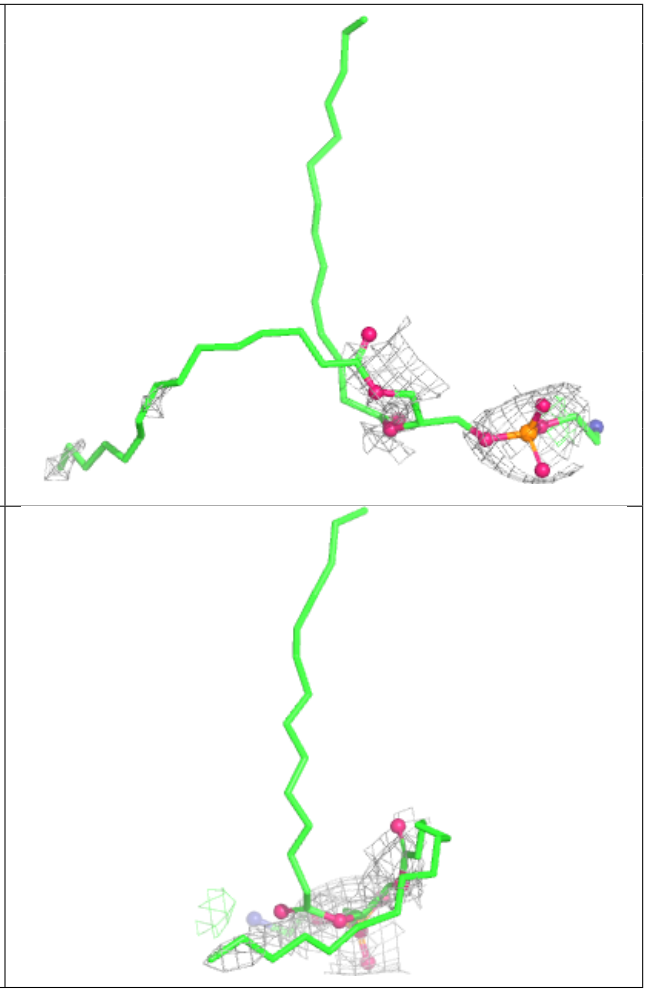
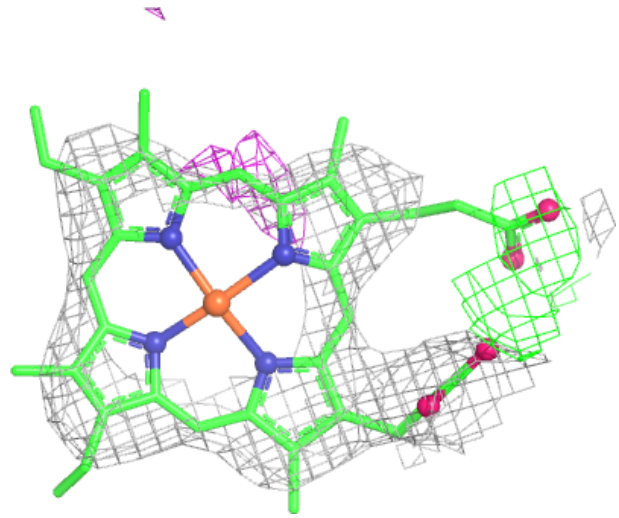
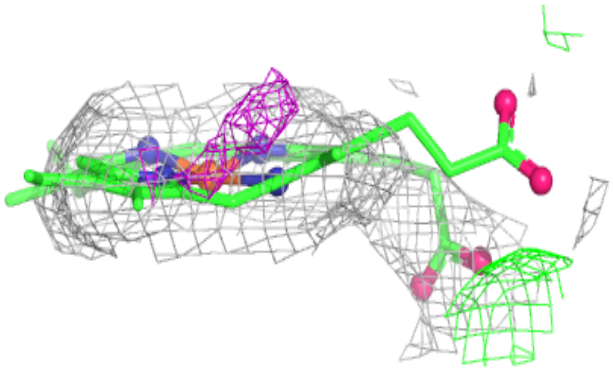
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

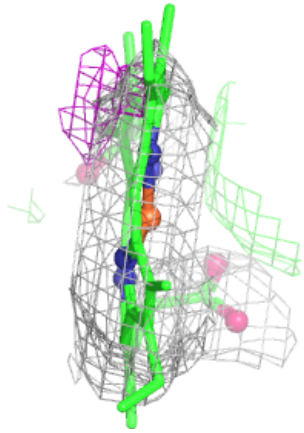


Electron density around HEM G 201:

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







Electron density around EPH D 201:

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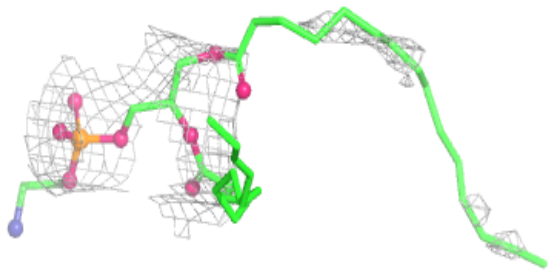
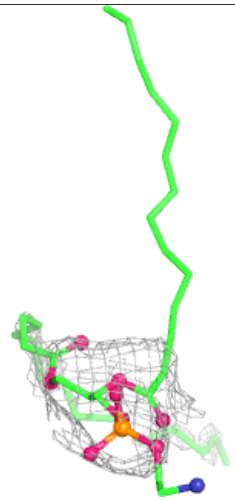
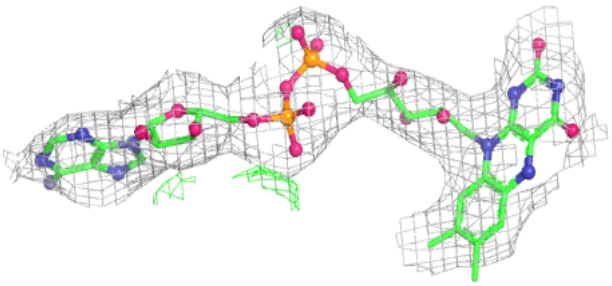
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

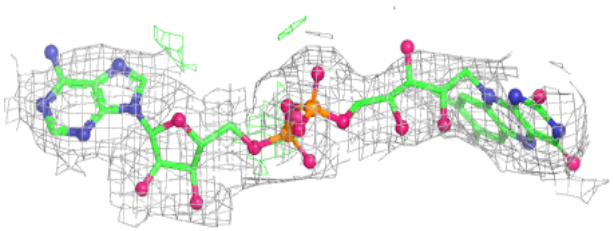


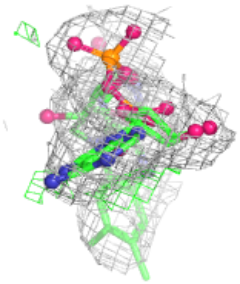


Electron density around FAD E 702:

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







Electron density around FAD A 702:

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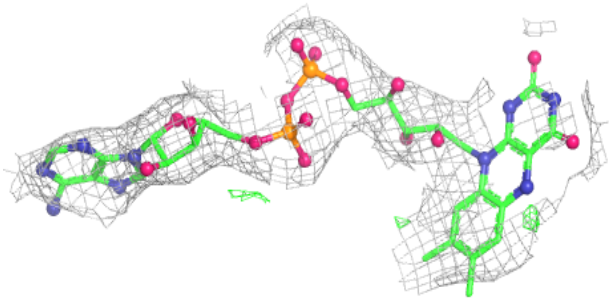
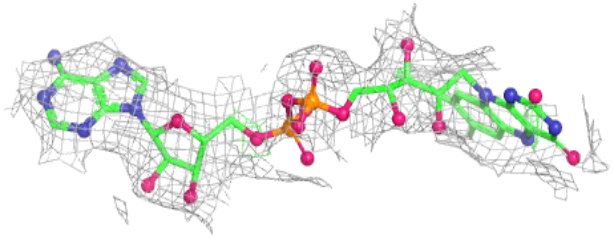
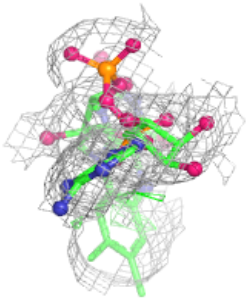
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEM C 201:

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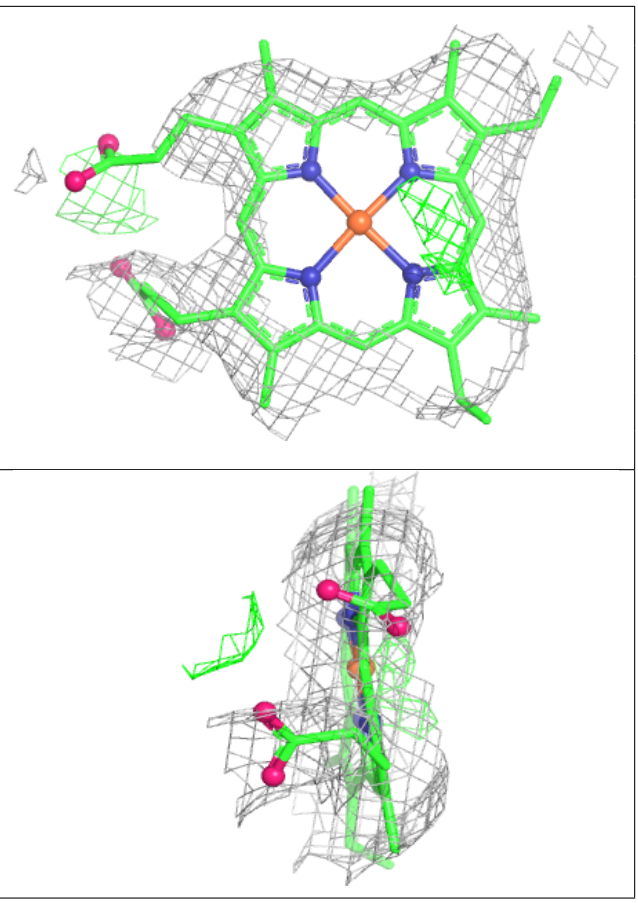
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.