Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2023 – 04:25 PM EDT

PDB ID	:	7UOR
Title	:	Crystal structure of cytochrome P450 enzyme CYP119 in complex with methyliridium(III) mesoporphyrin.
Authors	:	Pereira, J.H.; Bloomer, B.J.; Hartwig, J.F.; Adams, P.D.
Deposited on	:	2022-04-13
Resolution	:	3.16 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

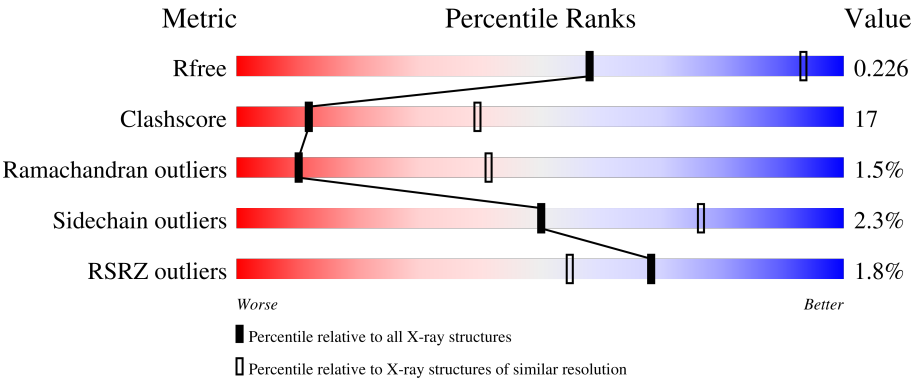
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.16 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}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	385	68% 28%
1	B	385	61% 36%
1	C	385	66% 29%
1	D	385	66% 29%
1	E	385	66% 29%

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Mol	Chain	Length	Quality of chain
1	F	385	2% 65% 31%

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
2	HIR	A	401	X	-	-	-
2	HIR	B	401	X	-	-	-
2	HIR	C	401	X	-	-	-
2	HIR	D	401	X	-	-	-
2	HIR	E	401	X	-	-	-
2	HIR	F	401	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19268 atoms, of which 114 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			3133	2005	545	579	4			
1	B	379	Total	C	N	O	S	0	0	0
			3133	2005	545	579	4			
1	C	379	Total	C	N	O	S	0	0	0
			3133	2005	545	579	4			
1	D	379	Total	C	N	O	S	0	0	0
			3133	2005	545	579	4			
1	E	379	Total	C	N	O	S	0	0	0
			3133	2005	545	579	4			
1	F	379	Total	C	N	O	S	0	0	0
			3133	2005	545	579	4			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP A0A0U3HD14
A	-15	LYS	-	expression tag	UNP A0A0U3HD14
A	-14	SER	-	expression tag	UNP A0A0U3HD14
A	-13	SER	-	expression tag	UNP A0A0U3HD14
A	-12	HIS	-	expression tag	UNP A0A0U3HD14
A	-11	HIS	-	expression tag	UNP A0A0U3HD14
A	-10	HIS	-	expression tag	UNP A0A0U3HD14
A	-9	HIS	-	expression tag	UNP A0A0U3HD14
A	-8	HIS	-	expression tag	UNP A0A0U3HD14
A	-7	HIS	-	expression tag	UNP A0A0U3HD14
A	-6	GLU	-	expression tag	UNP A0A0U3HD14
A	-5	ASN	-	expression tag	UNP A0A0U3HD14
A	-4	LEU	-	expression tag	UNP A0A0U3HD14
A	-3	TYR	-	expression tag	UNP A0A0U3HD14
A	-2	PHE	-	expression tag	UNP A0A0U3HD14
A	-1	GLN	-	expression tag	UNP A0A0U3HD14
A	0	SER	-	expression tag	UNP A0A0U3HD14

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ASN	-	expression tag	UNP A0A0U3HD14
A	155	TRP	LEU	engineered mutation	UNP A0A0U3HD14
A	213	GLY	THR	engineered mutation	UNP A0A0U3HD14
A	254	LEU	VAL	engineered mutation	UNP A0A0U3HD14
A	317	GLY	CYS	engineered mutation	UNP A0A0U3HD14
B	-16	MET	-	initiating methionine	UNP A0A0U3HD14
B	-15	LYS	-	expression tag	UNP A0A0U3HD14
B	-14	SER	-	expression tag	UNP A0A0U3HD14
B	-13	SER	-	expression tag	UNP A0A0U3HD14
B	-12	HIS	-	expression tag	UNP A0A0U3HD14
B	-11	HIS	-	expression tag	UNP A0A0U3HD14
B	-10	HIS	-	expression tag	UNP A0A0U3HD14
B	-9	HIS	-	expression tag	UNP A0A0U3HD14
B	-8	HIS	-	expression tag	UNP A0A0U3HD14
B	-7	HIS	-	expression tag	UNP A0A0U3HD14
B	-6	GLU	-	expression tag	UNP A0A0U3HD14
B	-5	ASN	-	expression tag	UNP A0A0U3HD14
B	-4	LEU	-	expression tag	UNP A0A0U3HD14
B	-3	TYR	-	expression tag	UNP A0A0U3HD14
B	-2	PHE	-	expression tag	UNP A0A0U3HD14
B	-1	GLN	-	expression tag	UNP A0A0U3HD14
B	0	SER	-	expression tag	UNP A0A0U3HD14
B	1	ASN	-	expression tag	UNP A0A0U3HD14
B	155	TRP	LEU	engineered mutation	UNP A0A0U3HD14
B	213	GLY	THR	engineered mutation	UNP A0A0U3HD14
B	254	LEU	VAL	engineered mutation	UNP A0A0U3HD14
B	317	GLY	CYS	engineered mutation	UNP A0A0U3HD14
C	-16	MET	-	initiating methionine	UNP A0A0U3HD14
C	-15	LYS	-	expression tag	UNP A0A0U3HD14
C	-14	SER	-	expression tag	UNP A0A0U3HD14
C	-13	SER	-	expression tag	UNP A0A0U3HD14
C	-12	HIS	-	expression tag	UNP A0A0U3HD14
C	-11	HIS	-	expression tag	UNP A0A0U3HD14
C	-10	HIS	-	expression tag	UNP A0A0U3HD14
C	-9	HIS	-	expression tag	UNP A0A0U3HD14
C	-8	HIS	-	expression tag	UNP A0A0U3HD14
C	-7	HIS	-	expression tag	UNP A0A0U3HD14
C	-6	GLU	-	expression tag	UNP A0A0U3HD14
C	-5	ASN	-	expression tag	UNP A0A0U3HD14
C	-4	LEU	-	expression tag	UNP A0A0U3HD14
C	-3	TYR	-	expression tag	UNP A0A0U3HD14
C	-2	PHE	-	expression tag	UNP A0A0U3HD14

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLN	-	expression tag	UNP A0A0U3HD14
C	0	SER	-	expression tag	UNP A0A0U3HD14
C	1	ASN	-	expression tag	UNP A0A0U3HD14
C	155	TRP	LEU	engineered mutation	UNP A0A0U3HD14
C	213	GLY	THR	engineered mutation	UNP A0A0U3HD14
C	254	LEU	VAL	engineered mutation	UNP A0A0U3HD14
C	317	GLY	CYS	engineered mutation	UNP A0A0U3HD14
D	-16	MET	-	initiating methionine	UNP A0A0U3HD14
D	-15	LYS	-	expression tag	UNP A0A0U3HD14
D	-14	SER	-	expression tag	UNP A0A0U3HD14
D	-13	SER	-	expression tag	UNP A0A0U3HD14
D	-12	HIS	-	expression tag	UNP A0A0U3HD14
D	-11	HIS	-	expression tag	UNP A0A0U3HD14
D	-10	HIS	-	expression tag	UNP A0A0U3HD14
D	-9	HIS	-	expression tag	UNP A0A0U3HD14
D	-8	HIS	-	expression tag	UNP A0A0U3HD14
D	-7	HIS	-	expression tag	UNP A0A0U3HD14
D	-6	GLU	-	expression tag	UNP A0A0U3HD14
D	-5	ASN	-	expression tag	UNP A0A0U3HD14
D	-4	LEU	-	expression tag	UNP A0A0U3HD14
D	-3	TYR	-	expression tag	UNP A0A0U3HD14
D	-2	PHE	-	expression tag	UNP A0A0U3HD14
D	-1	GLN	-	expression tag	UNP A0A0U3HD14
D	0	SER	-	expression tag	UNP A0A0U3HD14
D	1	ASN	-	expression tag	UNP A0A0U3HD14
D	155	TRP	LEU	engineered mutation	UNP A0A0U3HD14
D	213	GLY	THR	engineered mutation	UNP A0A0U3HD14
D	254	LEU	VAL	engineered mutation	UNP A0A0U3HD14
D	317	GLY	CYS	engineered mutation	UNP A0A0U3HD14
E	-16	MET	-	initiating methionine	UNP A0A0U3HD14
E	-15	LYS	-	expression tag	UNP A0A0U3HD14
E	-14	SER	-	expression tag	UNP A0A0U3HD14
E	-13	SER	-	expression tag	UNP A0A0U3HD14
E	-12	HIS	-	expression tag	UNP A0A0U3HD14
E	-11	HIS	-	expression tag	UNP A0A0U3HD14
E	-10	HIS	-	expression tag	UNP A0A0U3HD14
E	-9	HIS	-	expression tag	UNP A0A0U3HD14
E	-8	HIS	-	expression tag	UNP A0A0U3HD14
E	-7	HIS	-	expression tag	UNP A0A0U3HD14
E	-6	GLU	-	expression tag	UNP A0A0U3HD14
E	-5	ASN	-	expression tag	UNP A0A0U3HD14
E	-4	LEU	-	expression tag	UNP A0A0U3HD14

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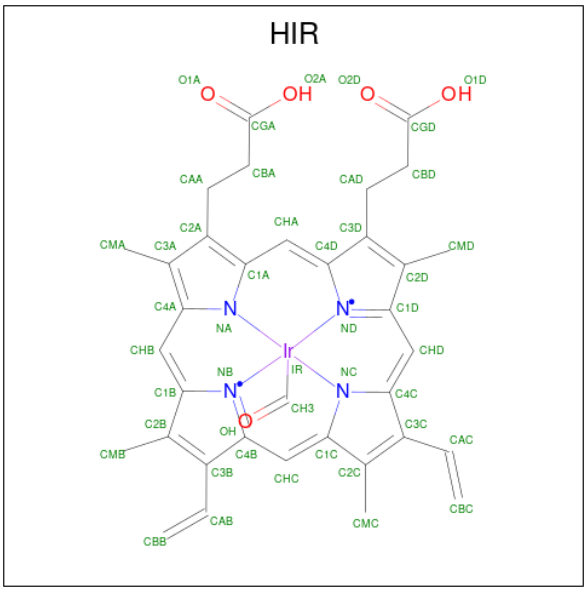
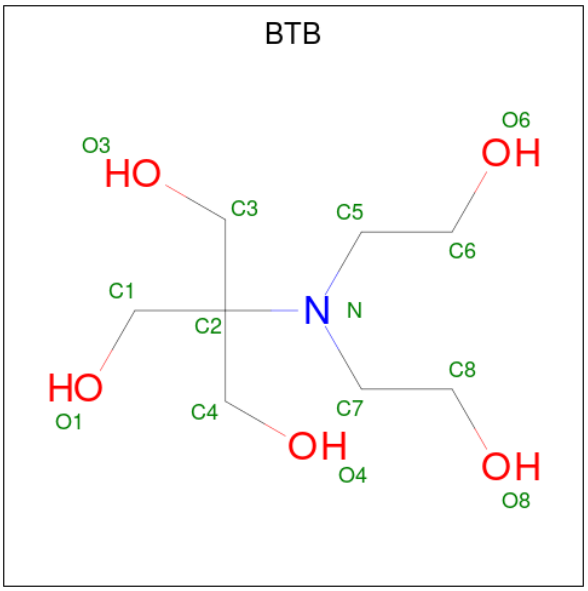
Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	TYR	-	expression tag	UNP A0A0U3HD14
E	-2	PHE	-	expression tag	UNP A0A0U3HD14
E	-1	GLN	-	expression tag	UNP A0A0U3HD14
E	0	SER	-	expression tag	UNP A0A0U3HD14
E	1	ASN	-	expression tag	UNP A0A0U3HD14
E	155	TRP	LEU	engineered mutation	UNP A0A0U3HD14
E	213	GLY	THR	engineered mutation	UNP A0A0U3HD14
E	254	LEU	VAL	engineered mutation	UNP A0A0U3HD14
E	317	GLY	CYS	engineered mutation	UNP A0A0U3HD14
F	-16	MET	-	initiating methionine	UNP A0A0U3HD14
F	-15	LYS	-	expression tag	UNP A0A0U3HD14
F	-14	SER	-	expression tag	UNP A0A0U3HD14
F	-13	SER	-	expression tag	UNP A0A0U3HD14
F	-12	HIS	-	expression tag	UNP A0A0U3HD14
F	-11	HIS	-	expression tag	UNP A0A0U3HD14
F	-10	HIS	-	expression tag	UNP A0A0U3HD14
F	-9	HIS	-	expression tag	UNP A0A0U3HD14
F	-8	HIS	-	expression tag	UNP A0A0U3HD14
F	-7	HIS	-	expression tag	UNP A0A0U3HD14
F	-6	GLU	-	expression tag	UNP A0A0U3HD14
F	-5	ASN	-	expression tag	UNP A0A0U3HD14
F	-4	LEU	-	expression tag	UNP A0A0U3HD14
F	-3	TYR	-	expression tag	UNP A0A0U3HD14
F	-2	PHE	-	expression tag	UNP A0A0U3HD14
F	-1	GLN	-	expression tag	UNP A0A0U3HD14
F	0	SER	-	expression tag	UNP A0A0U3HD14
F	1	ASN	-	expression tag	UNP A0A0U3HD14
F	155	TRP	LEU	engineered mutation	UNP A0A0U3HD14
F	213	GLY	THR	engineered mutation	UNP A0A0U3HD14
F	254	LEU	VAL	engineered mutation	UNP A0A0U3HD14
F	317	GLY	CYS	engineered mutation	UNP A0A0U3HD14

- Molecule 2 is methyliridium(III) mesoporphyrin (three-letter code: HIR) (formula: $C_{35}H_{32}IrN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Ir	N	O	0	0
			45	35	1	4	5		
2	B	1	Total	C	Ir	N	O	0	0
			45	35	1	4	5		
2	C	1	Total	C	Ir	N	O	0	0
			45	35	1	4	5		
2	D	1	Total	C	Ir	N	O	0	0
			45	35	1	4	5		
2	E	1	Total	C	Ir	N	O	0	0
			45	35	1	4	5		
2	F	1	Total	C	Ir	N	O	0	0
			45	35	1	4	5		

- Molecule 3 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			33	8	19	1	5		
3	B	1	Total	C	H	N	O	0	0
			33	8	19	1	5		
3	C	1	Total	C	H	N	O	0	0
			33	8	19	1	5		
3	D	1	Total	C	H	N	O	0	0
			33	8	19	1	5		
3	E	1	Total	C	H	N	O	0	0
			33	8	19	1	5		
3	F	1	Total	C	H	N	O	0	0
			33	8	19	1	5		

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

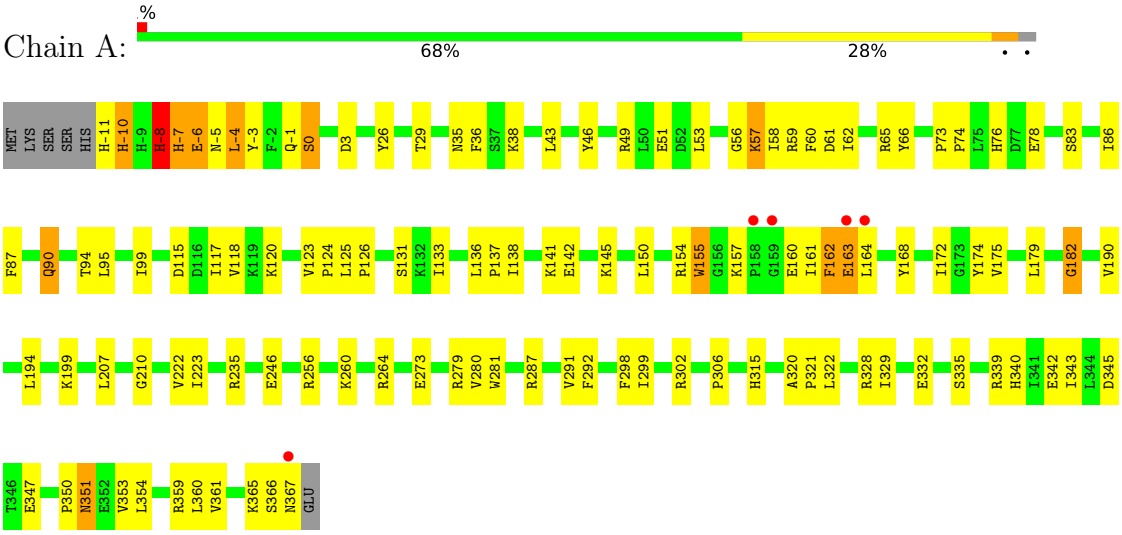
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ni	0	0
			1	1		
4	D	1	Total	Ni	0	0
			1	1		

3 Residue-property plots (i)

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

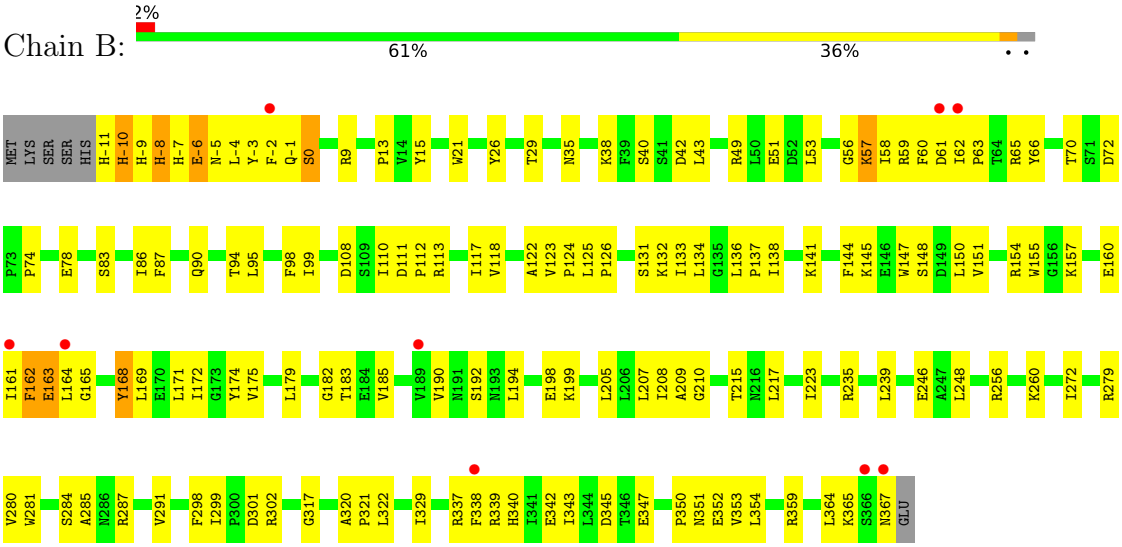
• Molecule 1: Cytochrome

Chain A:



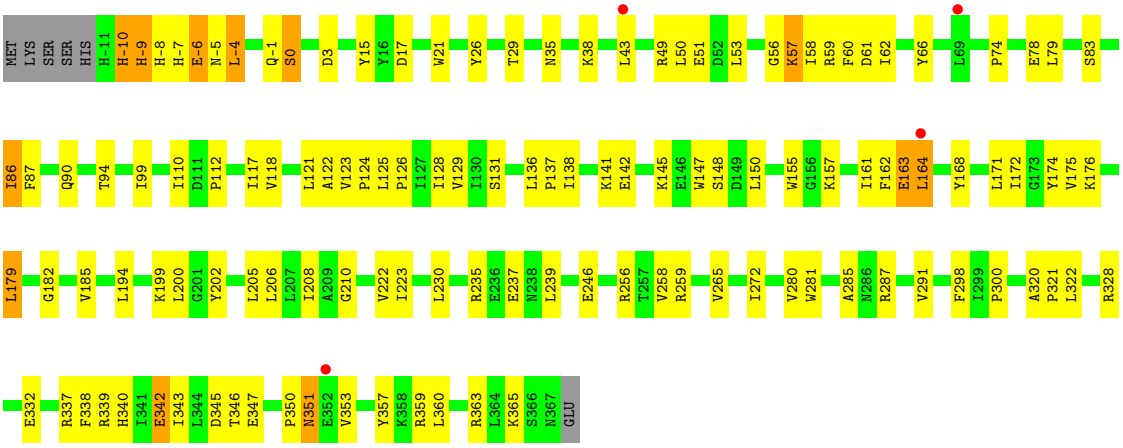
• Molecule 1: Cytochrome

Chain B:



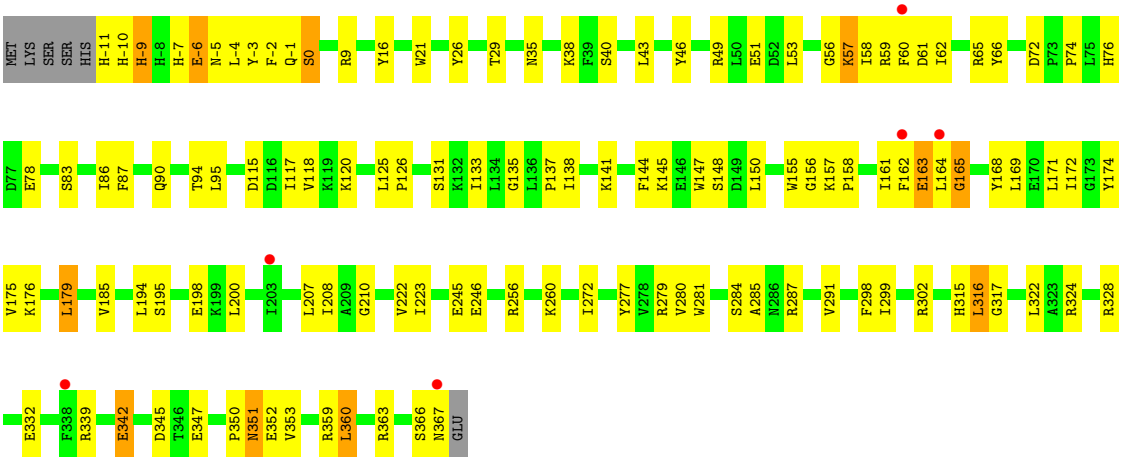
• Molecule 1: Cytochrome

Chain C:



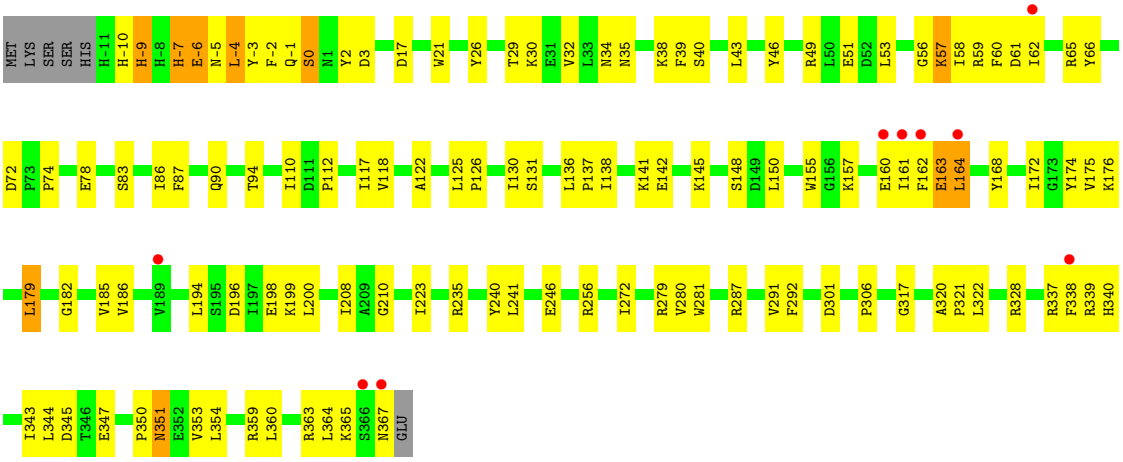
• Molecule 1: Cytochrome

Chain D:



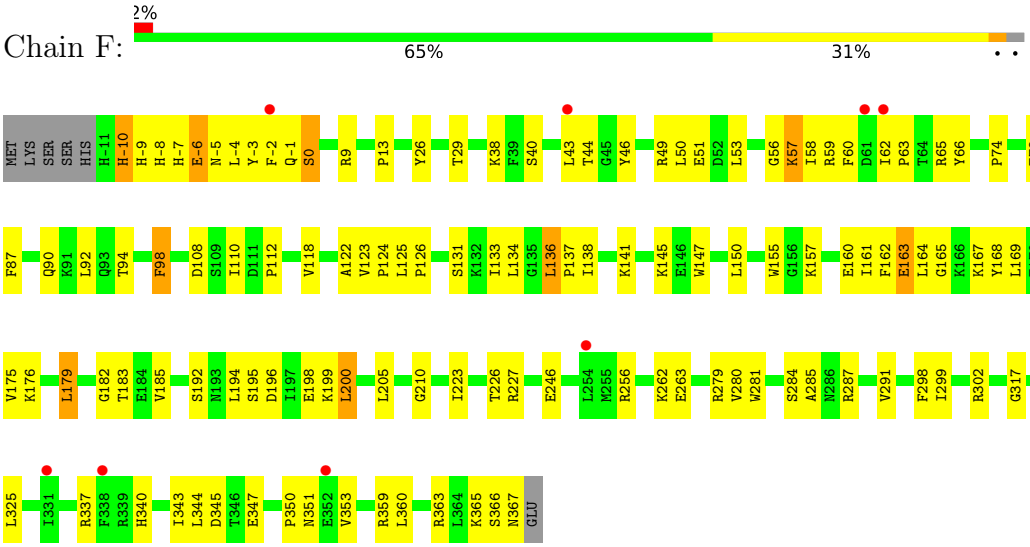
• Molecule 1: Cytochrome

Chain E:



• Molecule 1: Cytochrome

Chain F:


2%
65%
31%
MET LYS SER SER HIS H-11 H-10 H-9 H-8 H-7 E-6 N-5 L-4 Y-3 F-2 Q-1 S0 R9 P13 Y26 T29 K38 F39 S40 L43 T44 G45 Y46 R49 L50 E51 D52 L53 G56 K57 I58 R59 F60 D61 I62 P63 T64 R65 Y66 P74 E78 S83 I86
F87 Q90 K91 L92 Q93 T94 F98 D108 S109 I110 D111 P112 V118 A122 V123 P124 L125 P126 S131 K132 I133 L134 G135 L136 P137 I138 K141 K145 E146 W147 L150 W155 G156 K157 E160 I161 F162 E163 L164 G165 K166 K167 Y168 L169 E170 L171 I172 G173 Y174
V175 K176 L179 G182 T183 E184 V185 S192 N193 L194 S195 D196 I197 E198 K199 L200 L205 G210 I223 T226 R227 E246 L254 M255 R256 K262 E263 R279 V280 W281 S284 A285 N286 R287 V291 F298 I299 R302 G317 A320 P321 L322
L325 I331 R337 F338 R339 H340 I343 L344 D345 T346 E347 P350 N351 E352 V353 R359 L360 R363 L364 K365 S366 N367 GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	190.21Å 190.21Å 266.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.15 – 3.16 94.71 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.9 (60.15-3.16) 99.9 (94.71-3.16)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.20_4444, PHENIX 1.20_4444	Depositor
R, R_{free}	0.181 , 0.229 0.179 , 0.226	Depositor DCC
R_{free} test set	4001 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	83.7	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 64.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.000 for -1/2*h+1/2*k+1/2*l,1/2*h-1/2*k+1/2*l,h+k 0.000 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k 0.000 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.017 for -h,k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19268	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HIR, NI, BTB

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	0.58	0/3206	0.96	3/4334 (0.1%)
1	B	0.57	0/3206	0.94	2/4334 (0.0%)
1	C	0.57	0/3206	0.97	9/4334 (0.2%)
1	D	0.55	1/3206 (0.0%)	0.93	6/4334 (0.1%)
1	E	0.53	0/3206	0.91	5/4334 (0.1%)
1	F	0.47	0/3206	0.86	3/4334 (0.1%)
All	All	0.55	1/19236 (0.0%)	0.93	28/26004 (0.1%)

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
1	B	0	1
1	F	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	342	GLU	CG-CD	5.09	1.59	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	179	LEU	CA-CB-CG	8.27	134.33	115.30
1	C	200	LEU	CA-CB-CG	7.51	132.56	115.30
1	E	179	LEU	CA-CB-CG	7.50	132.55	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	179	LEU	CA-CB-CG	7.49	132.52	115.30
1	F	179	LEU	CA-CB-CG	7.45	132.44	115.30
1	D	360	LEU	CB-CG-CD2	-7.43	98.37	111.00
1	D	342	GLU	CA-CB-CG	6.30	127.27	113.40
1	D	165	GLY	C-N-CA	-6.20	106.20	121.70
1	F	200	LEU	CA-CB-CG	6.00	129.11	115.30
1	C	86	ILE	CG1-CB-CG2	-5.96	98.28	111.40
1	C	15	TYR	CB-CG-CD2	-5.94	117.43	121.00
1	E	2	TYR	CB-CG-CD2	5.92	124.55	121.00
1	A	155	TRP	N-CA-C	5.64	126.23	111.00
1	D	200	LEU	CA-CB-CG	5.63	128.25	115.30
1	D	316	LEU	CA-CB-CG	-5.56	102.52	115.30
1	B	15	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	C	79	LEU	CB-CG-CD2	-5.47	101.70	111.00
1	E	130	ILE	CG1-CB-CG2	-5.33	99.67	111.40
1	E	2	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	C	200	LEU	CB-CG-CD1	-5.24	102.09	111.00
1	E	164	LEU	CA-CB-CG	-5.22	103.29	115.30
1	C	342	GLU	CA-CB-CG	5.17	124.77	113.40
1	C	15	TYR	CB-CG-CD1	5.16	124.09	121.00
1	B	342	GLU	CA-CB-CG	5.12	124.66	113.40
1	A	342	GLU	CA-CB-CG	5.10	124.62	113.40
1	A	182	GLY	N-CA-C	5.07	125.77	113.10
1	C	164	LEU	CA-CB-CG	-5.07	103.65	115.30
1	F	136	LEU	CA-CB-CG	-5.01	103.77	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-8	HIS	Peptide
1	B	-8	HIS	Peptide
1	F	-8	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	3133	0	3129	97	0
1	B	3133	0	3129	132	0
1	C	3133	0	3129	111	0
1	D	3133	0	3129	108	0
1	E	3133	0	3129	120	0
1	F	3133	0	3129	104	0
2	A	45	0	0	2	0
2	B	45	0	0	2	0
2	C	45	0	0	4	0
2	D	45	0	0	1	0
2	E	45	0	0	2	0
2	F	45	0	0	3	0
3	A	14	19	19	2	0
3	B	14	19	19	2	0
3	C	14	19	19	3	0
3	D	14	19	19	2	0
3	E	14	19	19	1	0
3	F	14	19	19	2	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
All	All	19154	114	18888	659	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 17.

All (659) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ILE:HD11	1:B:185:VAL:HG21	1.16	1.08
1:D:345:ASP:OD2	1:D:359:ARG:NH2	1.88	1.07
1:F:345:ASP:OD2	1:F:359:ARG:NH2	1.90	1.05
1:A:345:ASP:OD2	1:A:359:ARG:NH2	1.90	1.05
1:D:86:ILE:HD11	1:D:185:VAL:HG21	1.37	1.03
1:F:83:SER:O	1:F:86:ILE:HG22	1.63	0.98
1:C:83:SER:O	1:C:86:ILE:HG22	1.64	0.97
1:B:345:ASP:OD2	1:B:359:ARG:NH2	1.95	0.97
1:B:340:HIS:HB2	1:B:365:LYS:HB2	1.44	0.97
1:E:345:ASP:OD2	1:E:359:ARG:NH2	1.97	0.96
1:C:345:ASP:OD2	1:C:359:ARG:NH2	1.98	0.96
1:E:86:ILE:HD11	1:E:185:VAL:HG21	1.47	0.95
1:A:83:SER:O	1:A:86:ILE:HG22	1.65	0.95
1:A:150:LEU:HD11	1:A:164:LEU:HD13	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:ARG:NH1	1:D:366:SER:O	2.00	0.93
1:F:137:PRO:O	1:F:174:TYR:OH	1.85	0.93
1:F:147:TRP:HB3	1:F:171:LEU:HD12	1.52	0.92
1:D:86:ILE:HD11	1:D:185:VAL:CG2	1.99	0.91
1:C:137:PRO:O	1:C:174:TYR:OH	1.89	0.89
1:D:83:SER:HB2	1:D:86:ILE:HD12	1.55	0.89
1:D:29:THR:HG23	1:D:280:VAL:CG1	2.03	0.88
1:A:157:LYS:NZ	1:A:163:GLU:OE1	2.07	0.87
1:F:176:LYS:HA	1:F:179:LEU:HD13	1.56	0.87
1:F:29:THR:HG23	1:F:280:VAL:CG1	2.03	0.87
1:D:168:TYR:CE2	1:D:172:ILE:HD11	2.09	0.87
1:F:29:THR:HG23	1:F:280:VAL:HG13	1.56	0.86
1:A:29:THR:HG23	1:A:280:VAL:CG1	2.06	0.86
1:E:347:GLU:OE1	1:E:359:ARG:HD3	1.76	0.85
1:E:29:THR:HG23	1:E:280:VAL:CG1	2.06	0.85
1:E:86:ILE:HD11	1:E:185:VAL:CG2	2.06	0.85
1:E:137:PRO:O	1:E:174:TYR:OH	1.94	0.85
1:B:137:PRO:O	1:B:174:TYR:OH	1.94	0.84
1:D:137:PRO:O	1:D:174:TYR:OH	1.96	0.83
1:A:49:ARG:HH21	1:A:58:ILE:HD13	1.41	0.83
1:B:29:THR:HG23	1:B:280:VAL:CG1	2.08	0.83
1:A:131:SER:HB2	1:A:138:ILE:HD12	1.61	0.83
1:E:168:TYR:CE2	1:E:172:ILE:HD11	2.14	0.82
1:B:86:ILE:HD11	1:B:185:VAL:CG2	2.07	0.82
1:E:176:LYS:HA	1:E:179:LEU:HD13	1.62	0.82
1:D:141:LYS:O	1:D:145:LYS:HG3	1.79	0.81
1:D:256:ARG:HD2	1:D:279:ARG:HD3	1.60	0.81
1:E:235:ARG:HH21	1:E:339:ARG:HH11	1.29	0.81
1:C:29:THR:HG23	1:C:280:VAL:CG1	2.11	0.81
1:B:86:ILE:CD1	1:B:185:VAL:HG21	2.06	0.80
1:C:131:SER:HB2	1:C:138:ILE:HD12	1.63	0.80
1:F:196:ASP:O	1:F:200:LEU:HD12	1.81	0.80
1:F:131:SER:HB2	1:F:138:ILE:HD12	1.63	0.79
1:D:86:ILE:CD1	1:D:185:VAL:HG21	2.11	0.79
1:B:147:TRP:HB3	1:B:171:LEU:HD12	1.65	0.78
1:D:40:SER:OG	1:D:72:ASP:OD2	2.02	0.78
1:A:29:THR:HG23	1:A:280:VAL:HG11	1.65	0.77
1:F:60:PHE:HA	1:F:161:ILE:HD12	1.63	0.77
1:D:56:GLY:O	1:D:57:LYS:HB2	1.82	0.77
1:A:154:ARG:CZ	1:A:164:LEU:HD11	2.14	0.77
1:B:111:ASP:OD1	1:B:113:ARG:HG2	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:LEU:HD22	1:D:198:GLU:OE1	1.85	0.77
1:B:168:TYR:CE1	1:B:172:ILE:HD11	2.20	0.76
1:D:87:PHE:HE1	1:D:322:LEU:HD22	1.51	0.76
1:D:277:TYR:CE2	1:E:-4:LEU:HD13	2.21	0.76
1:A:168:TYR:CE2	1:A:172:ILE:HD11	2.21	0.75
1:F:147:TRP:HB3	1:F:171:LEU:CD1	2.17	0.75
1:E:35:ASN:HD21	1:E:38:LYS:HD2	1.50	0.74
1:B:168:TYR:HE1	1:B:172:ILE:HD11	1.52	0.74
1:D:87:PHE:CE1	1:D:322:LEU:HD22	2.22	0.74
1:A:340:HIS:HB2	1:A:365:LYS:HG2	1.70	0.74
1:A:87:PHE:CE1	1:A:322:LEU:HD22	2.23	0.74
1:C:147:TRP:HB3	1:C:171:LEU:HD12	1.70	0.73
1:B:171:LEU:HD11	1:B:208:ILE:CD1	2.18	0.73
1:C:176:LYS:HA	1:C:179:LEU:HD13	1.70	0.73
1:F:165:GLY:HA2	1:F:169:LEU:HG	1.71	0.73
1:B:35:ASN:HD21	1:B:38:LYS:HD2	1.53	0.73
1:D:29:THR:HG23	1:D:280:VAL:HG11	1.71	0.72
1:F:176:LYS:HA	1:F:179:LEU:CD1	2.19	0.72
1:B:49:ARG:HH21	1:B:58:ILE:HD13	1.55	0.72
1:A:256:ARG:HD2	1:A:279:ARG:HD3	1.72	0.71
1:B:351:ASN:OD1	1:B:353:VAL:HG12	1.88	0.71
1:B:131:SER:HB2	1:B:138:ILE:HD12	1.69	0.71
1:D:131:SER:HB2	1:D:138:ILE:HD12	1.72	0.71
1:A:125:LEU:HB3	1:A:126:PRO:HD3	1.71	0.71
1:E:83:SER:HB2	1:E:86:ILE:HD12	1.71	0.71
1:A:137:PRO:O	1:A:174:TYR:OH	2.07	0.71
1:B:338:PHE:CD2	1:B:364:LEU:HD13	2.25	0.71
1:C:-6:GLU:HG2	1:C:-5:ASN:N	2.05	0.71
1:A:56:GLY:O	1:A:57:LYS:HB2	1.91	0.70
1:B:56:GLY:O	1:B:57:LYS:HB2	1.89	0.70
1:F:168:TYR:CE2	1:F:172:ILE:HD11	2.25	0.70
1:D:342:GLU:OE2	1:D:363:ARG:NH1	2.24	0.70
1:B:192:SER:OG	1:B:194:LEU:HD13	1.92	0.70
1:C:168:TYR:CE2	1:C:172:ILE:HD11	2.25	0.69
1:E:337:ARG:HG2	1:E:338:PHE:CZ	2.27	0.69
1:A:74:PRO:O	1:A:78:GLU:HG3	1.92	0.69
1:C:56:GLY:O	1:C:57:LYS:HB2	1.91	0.69
1:A:150:LEU:CD1	1:A:164:LEU:HD13	2.21	0.69
1:D:35:ASN:HD21	1:D:38:LYS:HD2	1.58	0.69
1:F:340:HIS:HB3	1:F:365:LYS:HG2	1.75	0.68
1:A:223:ILE:HD13	1:A:343:ILE:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:ASN:OD1	1:D:353:VAL:HG12	1.93	0.68
1:E:337:ARG:O	1:E:338:PHE:CD1	2.47	0.68
1:D:168:TYR:HE2	1:D:172:ILE:HD11	1.58	0.68
1:F:56:GLY:O	1:F:57:LYS:HB2	1.93	0.68
1:B:339:ARG:HG3	1:B:367:ASN:O	1.94	0.67
1:D:49:ARG:HH21	1:D:58:ILE:HD13	1.58	0.67
1:E:29:THR:HG23	1:E:280:VAL:HG13	1.76	0.67
1:E:256:ARG:HD2	1:E:279:ARG:HD3	1.76	0.67
1:B:83:SER:HB2	1:B:86:ILE:HD12	1.77	0.67
1:E:-6:GLU:HG2	1:E:-5:ASN:N	2.10	0.66
1:D:150:LEU:HD11	1:D:164:LEU:HD13	1.77	0.66
1:E:86:ILE:CD1	1:E:185:VAL:HG21	2.24	0.66
1:E:241:LEU:CD2	1:E:328:ARG:HD3	2.26	0.66
1:B:125:LEU:HB3	1:B:126:PRO:HD3	1.78	0.66
1:C:150:LEU:HD11	1:C:164:LEU:HD13	1.76	0.66
1:F:223:ILE:HD11	1:F:360:LEU:HD13	1.77	0.66
1:B:60:PHE:HA	1:B:161:ILE:HD12	1.77	0.65
1:C:168:TYR:CE2	1:C:172:ILE:CD1	2.79	0.65
1:B:338:PHE:CE2	1:B:364:LEU:HD13	2.31	0.65
1:D:299:ILE:HD12	1:D:302:ARG:NH2	2.11	0.65
1:E:241:LEU:HD23	1:E:328:ARG:HD3	1.78	0.65
1:C:171:LEU:HD11	1:C:208:ILE:CD1	2.27	0.64
1:D:277:TYR:HE2	1:E:-4:LEU:HD13	1.60	0.64
1:E:60:PHE:HA	1:E:161:ILE:HD12	1.79	0.64
1:F:350:PRO:O	1:F:351:ASN:HB2	1.98	0.64
1:E:87:PHE:CE1	1:E:322:LEU:HD22	2.33	0.64
1:B:147:TRP:HB3	1:B:171:LEU:CD1	2.27	0.64
1:A:87:PHE:HE1	1:A:322:LEU:HD22	1.60	0.64
1:B:87:PHE:HE1	1:B:322:LEU:HD22	1.62	0.63
1:C:29:THR:HG23	1:C:280:VAL:HG13	1.79	0.63
1:C:235:ARG:NE	1:C:339:ARG:NH1	2.45	0.63
1:F:125:LEU:HB3	1:F:126:PRO:HD3	1.79	0.63
1:F:168:TYR:HE2	1:F:172:ILE:HD11	1.62	0.63
1:C:342:GLU:OE2	1:C:363:ARG:NH1	2.31	0.63
1:E:292:PHE:CE1	1:E:306:PRO:HD2	2.34	0.63
1:D:115:ASP:OD2	1:D:120:LYS:NZ	2.30	0.63
1:E:168:TYR:HE2	1:E:172:ILE:HD11	1.61	0.63
1:E:168:TYR:CE2	1:E:172:ILE:CD1	2.82	0.63
1:B:-7:HIS:O	1:B:-6:GLU:CB	2.47	0.63
1:B:347:GLU:OE1	1:B:359:ARG:HD3	1.99	0.63
1:D:35:ASN:ND2	1:D:38:LYS:HD2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:ILE:HD12	1:D:157:LYS:O	1.99	0.63
1:E:56:GLY:O	1:E:57:LYS:HB2	1.99	0.63
1:D:29:THR:HG23	1:D:280:VAL:HG13	1.78	0.62
1:B:-3:TYR:O	1:C:157:LYS:NZ	2.33	0.62
1:A:347:GLU:OE1	1:A:359:ARG:HD3	1.98	0.62
1:C:87:PHE:CE1	1:C:322:LEU:HD22	2.34	0.62
1:D:21:TRP:CD1	1:D:272:ILE:HG23	2.34	0.62
1:D:74:PRO:O	1:D:78:GLU:HG3	1.99	0.62
1:F:192:SER:OG	1:F:194:LEU:HD13	1.99	0.62
1:A:60:PHE:HA	1:A:161:ILE:HD12	1.82	0.62
1:B:29:THR:HG23	1:B:280:VAL:HG11	1.80	0.62
1:B:108:ASP:OD1	1:B:337:ARG:NH2	2.24	0.62
1:C:347:GLU:OE1	1:C:359:ARG:HD3	2.00	0.62
1:B:99:ILE:HG22	1:B:329:ILE:HG21	1.81	0.62
1:D:-3:TYR:O	1:F:157:LYS:NZ	2.31	0.62
1:B:74:PRO:O	1:B:78:GLU:HG3	2.00	0.61
1:B:337:ARG:O	1:B:338:PHE:CD1	2.53	0.61
1:A:35:ASN:HD21	1:A:38:LYS:HD2	1.65	0.61
1:F:-6:GLU:HG2	1:F:-5:ASN:N	2.15	0.61
1:E:87:PHE:HE1	1:E:322:LEU:HD22	1.64	0.61
1:E:-1:GLN:O	1:E:3:ASP:HB2	2.00	0.61
1:F:63:PRO:HD2	1:F:168:TYR:OH	1.98	0.61
1:F:141:LYS:O	1:F:145:LYS:HG3	1.99	0.61
1:F:175:VAL:O	1:F:179:LEU:CD1	2.48	0.61
1:C:110:ILE:O	1:C:112:PRO:HD3	2.01	0.61
1:A:-11:HIS:O	1:A:-10:HIS:HB3	1.99	0.61
1:B:337:ARG:O	1:B:338:PHE:CG	2.54	0.61
1:B:-2:PHE:CE2	1:C:43:LEU:HD13	2.36	0.60
1:D:131:SER:HB2	1:D:138:ILE:CD1	2.31	0.60
1:A:118:VAL:HG23	1:A:360:LEU:HB3	1.82	0.60
1:C:256:ARG:HD3	1:C:281:TRP:CZ3	2.36	0.60
1:E:-7:HIS:O	1:E:-6:GLU:CB	2.48	0.60
1:E:35:ASN:ND2	1:E:38:LYS:HD2	2.15	0.60
1:E:49:ARG:HH21	1:E:58:ILE:HD13	1.65	0.60
1:C:86:ILE:HD12	1:C:185:VAL:HG11	1.83	0.60
1:F:299:ILE:HD12	1:F:302:ARG:NH2	2.17	0.60
1:D:-7:HIS:O	1:D:-6:GLU:CB	2.50	0.60
1:D:83:SER:HB2	1:D:86:ILE:CD1	2.29	0.59
1:E:29:THR:HG23	1:E:280:VAL:HG11	1.81	0.59
1:E:256:ARG:HG3	1:E:256:ARG:HH11	1.68	0.59
1:B:26:TYR:CG	1:B:291:VAL:HG21	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LYS:O	1:A:145:LYS:HG3	2.03	0.59
1:B:141:LYS:O	1:B:145:LYS:HG3	2.03	0.59
1:B:171:LEU:HD11	1:B:208:ILE:HD11	1.85	0.59
1:F:62:ILE:HD12	1:F:157:LYS:O	2.02	0.59
1:B:35:ASN:ND2	1:B:38:LYS:HD2	2.16	0.59
1:B:118:VAL:HA	1:B:122:ALA:HB3	1.85	0.59
1:D:350:PRO:O	1:D:351:ASN:CB	2.50	0.59
1:B:83:SER:HB2	1:B:86:ILE:CD1	2.33	0.58
1:D:-3:TYR:CE1	1:F:157:LYS:HD3	2.38	0.58
1:E:125:LEU:HB3	1:E:126:PRO:HD3	1.85	0.58
1:E:175:VAL:O	1:E:179:LEU:CD1	2.51	0.58
1:E:196:ASP:O	1:E:200:LEU:HD12	2.02	0.58
1:B:150:LEU:CD1	1:B:164:LEU:HD13	2.34	0.58
1:B:133:ILE:O	1:B:183:THR:HG21	2.02	0.58
1:E:256:ARG:HD3	1:E:281:TRP:CZ3	2.38	0.58
1:A:136:LEU:CD1	1:A:207:LEU:HD22	2.34	0.58
1:B:150:LEU:HD11	1:B:164:LEU:HD13	1.84	0.58
1:F:86:ILE:HG23	1:F:87:PHE:CD2	2.38	0.58
1:E:223:ILE:HD13	1:E:343:ILE:HD13	1.86	0.58
1:D:175:VAL:O	1:D:179:LEU:CD1	2.51	0.58
1:B:179:LEU:HD22	1:B:190:VAL:HG21	1.85	0.58
1:B:21:TRP:CD1	1:B:272:ILE:HG23	2.39	0.58
1:E:61:ASP:OD2	1:E:66:TYR:OH	2.20	0.58
1:F:256:ARG:NH1	1:F:279:ARG:HD2	2.18	0.58
1:C:142:GLU:HA	1:C:145:LYS:HG3	1.85	0.57
1:E:-7:HIS:O	1:E:-6:GLU:HB2	2.04	0.57
1:E:141:LYS:O	1:E:145:LYS:HG3	2.04	0.57
1:E:131:SER:HB2	1:E:138:ILE:HD12	1.84	0.57
1:D:256:ARG:HG3	1:D:256:ARG:HH11	1.68	0.57
1:F:74:PRO:O	1:F:78:GLU:HG3	2.05	0.57
1:F:87:PHE:HE1	1:F:322:LEU:HD22	1.68	0.57
1:B:87:PHE:CE1	1:B:322:LEU:HD22	2.39	0.57
1:D:156:GLY:O	1:D:158:PRO:HD3	2.04	0.57
1:E:351:ASN:OD1	1:E:353:VAL:HG12	2.04	0.57
1:A:366:SER:O	1:A:367:ASN:HB2	2.04	0.57
1:C:29:THR:HG23	1:C:280:VAL:HG11	1.87	0.57
1:C:340:HIS:HB2	1:C:365:LYS:HB2	1.86	0.57
1:A:35:ASN:ND2	1:A:38:LYS:HD2	2.20	0.57
1:C:320:ALA:HB3	1:C:321:PRO:HD3	1.86	0.56
1:D:168:TYR:CE2	1:D:172:ILE:CD1	2.86	0.56
1:B:-11:HIS:O	1:B:-10:HIS:HB3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-1:GLN:O	1:B:0:SER:CB	2.53	0.56
1:A:61:ASP:OD1	1:A:65:ARG:NH1	2.38	0.56
1:E:118:VAL:HA	1:E:122:ALA:HB3	1.87	0.56
1:F:347:GLU:OE1	1:F:359:ARG:HD3	2.05	0.56
1:C:246:GLU:OE1	1:C:246:GLU:HA	2.06	0.56
1:A:26:TYR:CG	1:A:291:VAL:HG21	2.40	0.56
1:B:-6:GLU:HG2	1:B:-5:ASN:N	2.21	0.56
1:E:110:ILE:O	1:E:112:PRO:HD3	2.04	0.56
1:E:340:HIS:HB2	1:E:365:LYS:HB2	1.87	0.56
1:A:-3:TYR:CZ	1:B:157:LYS:HD2	2.41	0.56
1:E:175:VAL:O	1:E:179:LEU:HD12	2.06	0.56
1:A:142:GLU:HA	1:A:145:LYS:HG3	1.88	0.56
1:F:175:VAL:O	1:F:179:LEU:HD12	2.06	0.56
1:A:351:ASN:OD1	1:A:351:ASN:C	2.44	0.56
1:F:-1:GLN:O	1:F:0:SER:CB	2.54	0.56
1:C:128:ILE:HD11	1:C:141:LYS:NZ	2.21	0.55
1:A:168:TYR:CE2	1:A:172:ILE:CD1	2.89	0.55
1:B:194:LEU:HB3	1:B:198:GLU:HB2	1.89	0.55
1:F:176:LYS:CA	1:F:179:LEU:HD13	2.32	0.55
1:D:147:TRP:HB3	1:D:171:LEU:HD12	1.88	0.55
1:E:61:ASP:O	1:E:161:ILE:HD11	2.06	0.55
1:E:351:ASN:OD1	1:E:351:ASN:C	2.45	0.55
1:F:162:PHE:O	1:F:164:LEU:N	2.39	0.55
1:F:133:ILE:O	1:F:183:THR:HG21	2.06	0.55
1:F:366:SER:O	1:F:367:ASN:HB2	2.07	0.55
1:B:29:THR:HG23	1:B:280:VAL:HG13	1.87	0.55
1:C:26:TYR:CD1	1:C:291:VAL:HG21	2.42	0.55
1:A:347:GLU:HB2	1:A:359:ARG:NH1	2.22	0.54
1:D:-1:GLN:O	1:D:0:SER:CB	2.54	0.54
1:A:-3:TYR:CE1	1:B:157:LYS:HD3	2.42	0.54
1:D:21:TRP:NE1	1:D:272:ILE:HG23	2.21	0.54
1:A:162:PHE:O	1:A:164:LEU:N	2.41	0.54
1:A:350:PRO:O	1:A:351:ASN:CB	2.56	0.54
1:B:-7:HIS:O	1:B:-6:GLU:HB2	2.06	0.54
1:D:171:LEU:HD11	1:D:208:ILE:CD1	2.37	0.54
1:A:246:GLU:HG3	1:A:298:PHE:CE2	2.43	0.54
1:A:299:ILE:HD12	1:A:302:ARG:NH2	2.21	0.54
1:C:-7:HIS:O	1:C:-6:GLU:CB	2.55	0.54
1:B:190:VAL:O	1:B:199:LYS:HE2	2.08	0.54
1:C:351:ASN:OD1	1:C:353:VAL:HG12	2.07	0.54
1:E:351:ASN:OD1	1:E:353:VAL:N	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ARG:HD3	1:B:281:TRP:CZ3	2.43	0.54
1:E:176:LYS:HA	1:E:179:LEU:CD1	2.36	0.54
1:C:175:VAL:O	1:C:179:LEU:CD1	2.56	0.53
1:F:147:TRP:CB	1:F:171:LEU:HD12	2.33	0.53
1:B:350:PRO:O	1:B:351:ASN:HB2	2.08	0.53
1:A:235:ARG:NH1	1:A:335:SER:O	2.42	0.53
1:A:351:ASN:OD1	1:A:353:VAL:HG12	2.09	0.53
1:E:235:ARG:HE	1:E:339:ARG:NH1	2.05	0.53
1:E:235:ARG:NH2	1:E:339:ARG:HD3	2.24	0.53
1:C:87:PHE:HE1	1:C:322:LEU:HD22	1.72	0.53
1:C:99:ILE:HG12	1:C:129:VAL:HG21	1.90	0.53
1:E:337:ARG:O	1:E:338:PHE:CG	2.61	0.53
1:B:-10:HIS:HE1	1:B:-8:HIS:CE1	2.26	0.53
1:C:74:PRO:O	1:C:78:GLU:HG3	2.07	0.53
1:E:32:VAL:HG13	1:E:39:PHE:CG	2.44	0.53
1:D:-6:GLU:HG2	1:D:-5:ASN:N	2.23	0.53
1:B:122:ALA:C	1:B:215:THR:HG23	2.29	0.53
1:C:147:TRP:HB3	1:C:171:LEU:CD1	2.37	0.53
1:D:43:LEU:HD13	1:E:-2:PHE:CE2	2.44	0.53
1:D:245:GLU:OE2	1:D:324:ARG:NE	2.36	0.53
1:A:328:ARG:HD3	1:A:332:GLU:OE2	2.09	0.53
1:B:256:ARG:HD2	1:B:279:ARG:HD3	1.91	0.53
1:B:340:HIS:HB2	1:B:365:LYS:CB	2.28	0.53
1:C:194:LEU:O	1:C:199:LYS:HE3	2.09	0.52
1:C:210:GLY:HA3	2:C:401:HIR:C2C	2.39	0.52
1:D:350:PRO:O	1:D:351:ASN:HB2	2.09	0.52
1:A:61:ASP:O	1:A:161:ILE:HD11	2.09	0.52
2:C:401:HIR:CBB	2:C:401:HIR:CMB	2.87	0.52
1:D:347:GLU:HB2	1:D:359:ARG:NH1	2.23	0.52
1:A:-6:GLU:HG2	1:A:-5:ASN:N	2.23	0.52
1:C:26:TYR:CG	1:C:291:VAL:HG21	2.45	0.52
1:F:51:GLU:C	1:F:53:LEU:H	2.13	0.52
1:B:123:VAL:N	1:B:124:PRO:HD2	2.25	0.52
1:B:179:LEU:HD22	1:B:190:VAL:CG2	2.38	0.52
1:C:351:ASN:OD1	1:C:351:ASN:C	2.48	0.52
1:D:43:LEU:CD2	1:D:260:LYS:HB2	2.40	0.52
1:A:-7:HIS:O	1:A:-6:GLU:CB	2.57	0.52
1:D:-10:HIS:HE1	1:E:-10:HIS:NE2	2.08	0.52
1:D:16:TYR:HB2	1:D:21:TRP:CH2	2.45	0.52
1:D:175:VAL:O	1:D:179:LEU:HD13	2.10	0.52
1:B:26:TYR:CD1	1:B:291:VAL:HG21	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:LEU:O	1:D:195:SER:HB3	2.09	0.52
1:B:111:ASP:OD1	1:B:113:ARG:CG	2.57	0.51
1:B:165:GLY:HA2	1:B:169:LEU:HG	1.92	0.51
1:C:123:VAL:HB	1:C:124:PRO:HD3	1.92	0.51
1:C:340:HIS:HB2	1:C:365:LYS:HG2	1.92	0.51
1:D:60:PHE:HA	1:D:161:ILE:HD12	1.92	0.51
1:F:165:GLY:O	1:F:169:LEU:HB2	2.10	0.51
1:A:76:HIS:CD2	1:A:315:HIS:CE1	2.99	0.51
1:B:147:TRP:CB	1:B:171:LEU:HD12	2.39	0.51
1:B:144:PHE:HZ	1:B:207:LEU:HG	1.74	0.51
1:B:210:GLY:HA3	2:B:401:HIR:C2C	2.41	0.51
1:F:351:ASN:OD1	1:F:353:VAL:HG12	2.10	0.51
1:B:9:ARG:HD3	1:B:284:SER:OG	2.09	0.51
1:D:26:TYR:CG	1:D:291:VAL:HG21	2.46	0.51
1:E:148:SER:HA	1:E:208:ILE:HG21	1.92	0.51
1:D:-7:HIS:O	1:D:-6:GLU:HB2	2.10	0.51
1:D:171:LEU:HD11	1:D:208:ILE:HD11	1.92	0.51
1:C:175:VAL:O	1:C:179:LEU:HD12	2.11	0.51
1:D:-10:HIS:HE1	1:E:-10:HIS:CE1	2.28	0.51
1:D:26:TYR:CD1	1:D:291:VAL:HG21	2.45	0.51
1:D:256:ARG:HD3	1:D:281:TRP:CH2	2.46	0.51
1:A:320:ALA:HB3	1:A:321:PRO:HD3	1.91	0.51
1:C:131:SER:HB2	1:C:138:ILE:CD1	2.39	0.51
1:F:87:PHE:CE1	1:F:322:LEU:HD22	2.46	0.51
1:F:157:LYS:HA	1:F:157:LYS:HE3	1.92	0.51
1:A:131:SER:HB2	1:A:138:ILE:CD1	2.38	0.51
1:E:350:PRO:O	1:E:351:ASN:CB	2.57	0.51
1:C:60:PHE:HA	1:C:161:ILE:HD12	1.93	0.50
1:D:176:LYS:HA	1:D:179:LEU:HD13	1.93	0.50
1:F:246:GLU:HG3	1:F:298:PHE:CE2	2.46	0.50
1:A:95:LEU:HD11	1:A:133:ILE:HG12	1.93	0.50
1:F:194:LEU:HD23	1:F:198:GLU:HB3	1.92	0.50
1:C:125:LEU:HB3	1:C:126:PRO:HD3	1.92	0.50
1:E:162:PHE:O	1:E:164:LEU:N	2.44	0.50
1:C:-1:GLN:O	1:C:0:SER:CB	2.58	0.50
1:F:26:TYR:CD1	1:F:291:VAL:HG21	2.47	0.50
1:A:353:VAL:HG13	1:A:354:LEU:HG	1.93	0.50
1:C:61:ASP:OD2	1:C:66:TYR:OH	2.29	0.50
1:D:118:VAL:HG23	1:D:360:LEU:HB3	1.94	0.50
1:A:-3:TYR:CE1	1:B:157:LYS:CD	2.95	0.50
1:B:9:ARG:O	1:B:13:PRO:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-2:PHE:CE2	1:F:43:LEU:HD13	2.46	0.49
1:A:136:LEU:HD12	1:A:207:LEU:HD22	1.94	0.49
1:C:118:VAL:HA	1:C:122:ALA:HB3	1.93	0.49
1:E:90:GLN:O	1:E:94:THR:HG23	2.12	0.49
1:C:142:GLU:HG2	1:C:145:LYS:HE3	1.95	0.49
1:C:235:ARG:CZ	1:C:339:ARG:HH11	2.25	0.49
1:D:61:ASP:O	1:D:161:ILE:HD11	2.13	0.49
1:A:256:ARG:HD3	1:A:281:TRP:CZ3	2.47	0.49
1:B:90:GLN:O	1:B:94:THR:HG23	2.13	0.49
1:B:320:ALA:HB3	1:B:321:PRO:HD3	1.95	0.49
1:F:-10:HIS:ND1	1:F:-9:HIS:N	2.59	0.49
1:F:223:ILE:O	1:F:227:ARG:HG3	2.13	0.49
1:B:350:PRO:O	1:B:351:ASN:CB	2.61	0.49
1:D:157:LYS:HD3	1:E:-3:TYR:CE1	2.47	0.49
1:E:26:TYR:CG	1:E:291:VAL:HG21	2.47	0.49
1:A:154:ARG:NE	1:A:164:LEU:HD11	2.28	0.49
1:C:-4:LEU:HD12	1:C:-1:GLN:OE1	2.13	0.49
1:C:230:LEU:HD22	1:C:300:PRO:HG3	1.93	0.49
1:D:150:LEU:CD1	1:D:164:LEU:HD13	2.42	0.49
1:E:148:SER:HA	1:E:208:ILE:CG2	2.42	0.49
1:E:338:PHE:CD1	1:E:364:LEU:HB3	2.48	0.49
1:F:9:ARG:HD3	1:F:284:SER:OG	2.13	0.49
1:E:339:ARG:HG2	1:E:367:ASN:O	2.12	0.49
1:E:347:GLU:HB2	1:E:359:ARG:NH1	2.28	0.49
1:B:62:ILE:HD12	1:B:157:LYS:O	2.13	0.48
1:C:256:ARG:HH11	1:C:256:ARG:HG3	1.78	0.48
1:E:320:ALA:HB3	1:E:321:PRO:HD3	1.94	0.48
1:B:154:ARG:O	1:B:157:LYS:HG2	2.13	0.48
3:B:402:BTB:H52	3:B:402:BTB:O1	2.13	0.48
1:F:98:PHE:CD1	1:F:98:PHE:C	2.86	0.48
1:A:-1:GLN:O	1:A:0:SER:CB	2.60	0.48
1:A:43:LEU:CD2	1:A:260:LYS:HB2	2.43	0.48
3:A:402:BTB:H62	3:A:402:BTB:H71	1.59	0.48
1:B:148:SER:HA	1:B:208:ILE:HG21	1.95	0.48
1:C:26:TYR:HA	1:C:285:ALA:HB1	1.96	0.48
1:A:246:GLU:OE1	1:A:246:GLU:HA	2.12	0.48
1:C:35:ASN:HD21	1:C:38:LYS:HD2	1.77	0.48
1:D:46:TYR:CD1	1:D:66:TYR:HD1	2.30	0.48
1:C:49:ARG:HH21	1:C:58:ILE:HD13	1.78	0.48
1:F:29:THR:HG23	1:F:280:VAL:HG11	1.92	0.48
1:C:150:LEU:CD1	1:C:164:LEU:HD13	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:LEU:HB3	1:D:126:PRO:HD3	1.96	0.48
1:C:-10:HIS:O	1:C:-9:HIS:HB3	2.14	0.48
1:C:51:GLU:C	1:C:53:LEU:H	2.16	0.48
1:D:256:ARG:HD2	1:D:279:ARG:CD	2.37	0.48
1:F:320:ALA:HB3	1:F:321:PRO:HD3	1.96	0.48
1:C:246:GLU:HG3	1:C:298:PHE:CE2	2.49	0.48
1:C:256:ARG:HD3	1:C:281:TRP:CH2	2.49	0.48
1:E:-1:GLN:O	1:E:0:SER:CB	2.62	0.48
1:B:61:ASP:OD2	1:B:66:TYR:OH	2.31	0.48
1:D:210:GLY:HA3	2:D:401:HIR:C2C	2.44	0.48
1:F:108:ASP:OD1	1:F:337:ARG:NH1	2.36	0.48
1:A:90:GLN:O	1:A:94:THR:HG23	2.14	0.47
1:D:51:GLU:C	1:D:53:LEU:H	2.17	0.47
1:E:338:PHE:CZ	1:E:364:LEU:HD13	2.49	0.47
1:B:162:PHE:O	1:B:164:LEU:N	2.47	0.47
1:D:53:LEU:HD23	1:D:53:LEU:HA	1.49	0.47
1:F:-7:HIS:O	1:F:-6:GLU:CB	2.62	0.47
1:B:168:TYR:CE1	1:B:172:ILE:CD1	2.94	0.47
1:B:-10:HIS:HE1	1:B:-8:HIS:NE2	2.12	0.47
1:C:38:LYS:HB3	1:C:265:VAL:HG11	1.96	0.47
1:D:162:PHE:O	1:D:164:LEU:N	2.47	0.47
1:F:118:VAL:HG23	1:F:360:LEU:HB3	1.97	0.47
1:F:223:ILE:HD11	1:F:360:LEU:CD1	2.44	0.47
1:C:-1:GLN:O	1:C:3:ASP:HB2	2.15	0.47
1:B:21:TRP:NE1	1:B:272:ILE:HG23	2.29	0.47
3:D:402:BTB:O1	3:D:402:BTB:H52	2.13	0.47
1:F:210:GLY:HA3	2:F:401:HIR:CMC	2.43	0.47
1:A:51:GLU:C	1:A:53:LEU:H	2.17	0.47
1:A:223:ILE:HD11	1:A:360:LEU:HD13	1.97	0.47
1:A:256:ARG:HG3	1:A:256:ARG:HH11	1.79	0.47
1:C:128:ILE:HD11	1:C:141:LYS:HZ3	1.79	0.47
1:C:205:LEU:HD21	2:C:401:HIR:CMD	2.45	0.47
1:C:350:PRO:O	1:C:351:ASN:CB	2.61	0.47
1:D:90:GLN:O	1:D:94:THR:HG23	2.14	0.47
1:E:40:SER:OG	1:E:72:ASP:OD2	2.22	0.47
1:F:-1:GLN:O	1:F:0:SER:HB3	2.15	0.47
1:F:90:GLN:O	1:F:94:THR:HG23	2.14	0.47
1:A:62:ILE:HD12	1:A:157:LYS:O	2.15	0.47
1:A:86:ILE:HG23	1:A:87:PHE:CD2	2.50	0.47
1:B:-1:GLN:O	1:B:0:SER:HB3	2.15	0.47
1:D:157:LYS:HE3	1:D:157:LYS:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:GLU:HG3	1:D:298:PHE:CE2	2.49	0.47
1:A:117:ILE:HD11	1:A:222:VAL:HG11	1.96	0.47
1:B:61:ASP:OD1	1:B:65:ARG:NH1	2.48	0.47
1:B:134:LEU:HA	1:B:183:THR:OG1	2.15	0.47
1:C:-6:GLU:CG	1:C:-5:ASN:N	2.76	0.47
1:C:351:ASN:OD1	1:C:353:VAL:N	2.38	0.47
1:C:62:ILE:HD12	1:C:157:LYS:O	2.15	0.47
1:B:148:SER:HA	1:B:208:ILE:CG2	2.46	0.46
1:B:223:ILE:HD13	1:B:343:ILE:HD13	1.96	0.46
1:C:246:GLU:HG3	1:C:298:PHE:CZ	2.50	0.46
1:C:346:THR:HG22	1:C:360:LEU:CD1	2.45	0.46
1:A:179:LEU:HD22	1:A:190:VAL:HG21	1.97	0.46
1:E:194:LEU:O	1:E:199:LYS:HE3	2.15	0.46
1:B:175:VAL:O	1:B:179:LEU:HG	2.15	0.46
2:B:401:HIR:CBB	2:B:401:HIR:CMB	2.94	0.46
1:D:76:HIS:CD2	1:D:315:HIS:CE1	3.03	0.46
1:D:366:SER:O	1:D:367:ASN:HB2	2.16	0.46
1:E:62:ILE:HD12	1:E:157:LYS:O	2.15	0.46
1:A:179:LEU:HD22	1:A:190:VAL:CG2	2.44	0.46
3:B:402:BTB:H62	3:B:402:BTB:H71	1.65	0.46
1:E:74:PRO:O	1:E:78:GLU:HG3	2.15	0.46
1:B:113:ARG:HG2	1:B:113:ARG:H	1.53	0.46
1:C:237:GLU:HB2	1:C:239:LEU:HG	1.97	0.46
1:B:168:TYR:HD1	1:B:168:TYR:O	1.97	0.46
1:C:168:TYR:HE2	1:C:172:ILE:HD11	1.79	0.46
1:D:135:GLY:O	1:D:137:PRO:HD3	2.15	0.46
1:F:350:PRO:O	1:F:351:ASN:CB	2.60	0.46
1:C:61:ASP:O	1:C:161:ILE:HD11	2.15	0.46
1:E:157:LYS:HD2	1:F:-3:TYR:CZ	2.51	0.46
1:F:26:TYR:HA	1:F:285:ALA:HB1	1.98	0.46
1:F:86:ILE:HD12	1:F:185:VAL:HG11	1.97	0.46
3:F:402:BTB:H62	3:F:402:BTB:H71	1.68	0.46
1:C:176:LYS:HA	1:C:179:LEU:CD1	2.42	0.46
1:E:117:ILE:HD12	1:E:117:ILE:HG23	1.71	0.46
1:A:-4:LEU:H	1:A:-4:LEU:HD12	1.80	0.46
1:F:157:LYS:HE3	1:F:157:LYS:CA	2.45	0.46
1:A:-8:HIS:CD2	1:B:-10:HIS:CE1	3.04	0.46
1:A:46:TYR:CD1	1:A:66:TYR:HD1	2.34	0.46
1:A:292:PHE:CE1	1:A:306:PRO:HD2	2.51	0.46
1:C:35:ASN:ND2	1:C:38:LYS:HD2	2.31	0.46
1:E:246:GLU:HA	1:E:246:GLU:OE1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:337:ARG:C	1:E:338:PHE:CG	2.90	0.45
1:A:194:LEU:O	1:A:199:LYS:HE3	2.16	0.45
1:B:42:ASP:HA	1:B:70:THR:O	2.16	0.45
1:E:235:ARG:NH2	1:E:339:ARG:HH11	2.07	0.45
1:F:194:LEU:HB3	1:F:198:GLU:HB2	1.97	0.45
1:B:351:ASN:HD21	1:B:353:VAL:CG1	2.30	0.45
1:E:118:VAL:HG23	1:E:360:LEU:HB3	1.98	0.45
1:F:131:SER:HB2	1:F:138:ILE:CD1	2.40	0.45
1:D:351:ASN:OD1	1:D:352:GLU:N	2.49	0.45
1:E:337:ARG:HG2	1:E:338:PHE:CE2	2.52	0.45
1:F:256:ARG:HG3	1:F:256:ARG:HH11	1.82	0.45
1:F:256:ARG:HD3	1:F:281:TRP:CZ3	2.51	0.45
1:E:142:GLU:HA	1:E:145:LYS:HG3	1.98	0.45
1:F:92:LEU:HB3	1:F:325:LEU:HD22	1.97	0.45
1:F:194:LEU:O	1:F:199:LYS:HE3	2.16	0.45
1:C:168:TYR:CZ	1:C:172:ILE:HD11	2.52	0.45
1:E:17:ASP:OD1	1:E:17:ASP:C	2.55	0.45
1:E:61:ASP:OD1	1:E:65:ARG:NH1	2.49	0.45
1:E:210:GLY:HA3	2:E:401:HIR:CMC	2.46	0.45
1:F:160:GLU:O	1:F:163:GLU:HG3	2.17	0.45
1:A:29:THR:HG23	1:A:280:VAL:HG13	1.97	0.45
1:A:168:TYR:HE2	1:A:172:ILE:HD11	1.77	0.45
1:C:117:ILE:HD11	1:C:222:VAL:HG11	1.98	0.45
1:D:117:ILE:CD1	1:D:222:VAL:HG11	2.46	0.45
1:E:241:LEU:HD21	1:E:328:ARG:HD3	1.98	0.45
1:A:115:ASP:OD2	1:A:120:LYS:NZ	2.41	0.45
1:E:353:VAL:HG13	1:E:354:LEU:HG	1.98	0.45
1:A:117:ILE:CD1	1:A:222:VAL:HG11	2.48	0.44
1:B:63:PRO:HD2	1:B:168:TYR:OH	2.16	0.44
1:B:157:LYS:HE3	1:B:157:LYS:HA	1.99	0.44
1:B:256:ARG:HG3	1:B:256:ARG:HH11	1.81	0.44
1:E:235:ARG:HG2	1:E:240:TYR:OH	2.16	0.44
1:E:46:TYR:CE1	1:E:66:TYR:HB3	2.52	0.44
1:E:223:ILE:HD11	1:E:360:LEU:HD13	1.99	0.44
1:F:53:LEU:O	1:F:195:SER:HB3	2.18	0.44
1:D:-10:HIS:CE1	1:E:-10:HIS:NE2	2.84	0.44
1:A:162:PHE:O	1:A:163:GLU:C	2.56	0.44
1:B:43:LEU:CD2	1:B:260:LYS:HB2	2.48	0.44
1:B:53:LEU:HD23	1:B:53:LEU:HA	1.59	0.44
3:C:402:BTB:H52	3:C:402:BTB:O1	2.17	0.44
1:D:148:SER:HA	1:D:208:ILE:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:GLU:C	1:E:53:LEU:H	2.21	0.44
1:E:210:GLY:HA3	2:E:401:HIR:C2C	2.47	0.44
1:B:111:ASP:OD1	1:B:113:ARG:CD	2.66	0.44
1:C:328:ARG:HD3	1:C:332:GLU:OE2	2.17	0.44
1:B:-3:TYR:CE1	1:C:157:LYS:HD3	2.52	0.44
1:C:-4:LEU:HD12	1:C:-4:LEU:H	1.82	0.44
1:F:351:ASN:HD21	1:F:353:VAL:HG12	1.83	0.44
3:F:402:BTB:O1	3:F:402:BTB:H52	2.17	0.44
1:A:26:TYR:CD1	1:A:291:VAL:HG21	2.53	0.44
1:F:46:TYR:CD1	1:F:66:TYR:HD1	2.36	0.44
1:F:162:PHE:O	1:F:163:GLU:C	2.55	0.44
1:A:46:TYR:CE1	1:A:66:TYR:HB3	2.52	0.43
1:B:110:ILE:O	1:B:112:PRO:HD3	2.18	0.43
1:E:157:LYS:NZ	1:F:-3:TYR:O	2.48	0.43
1:A:53:LEU:HA	1:A:53:LEU:HD23	1.64	0.43
1:C:223:ILE:HD13	1:C:343:ILE:HD13	1.99	0.43
1:F:118:VAL:HA	1:F:122:ALA:HB3	1.99	0.43
1:A:264:ARG:HE	1:A:273:GLU:CD	2.22	0.43
1:A:366:SER:O	1:A:367:ASN:CB	2.64	0.43
2:A:401:HIR:CBB	2:A:401:HIR:CMB	2.96	0.43
1:B:123:VAL:N	1:B:124:PRO:CD	2.82	0.43
1:F:50:LEU:O	1:F:53:LEU:HB2	2.18	0.43
1:E:136:LEU:HA	1:E:136:LEU:HD23	1.76	0.43
1:F:53:LEU:HD23	1:F:53:LEU:HA	1.65	0.43
1:D:144:PHE:HZ	1:D:207:LEU:HG	1.83	0.43
1:F:134:LEU:C	1:F:183:THR:HG23	2.39	0.43
1:D:162:PHE:O	1:D:163:GLU:C	2.57	0.43
1:E:185:VAL:HG13	1:E:186:VAL:N	2.34	0.43
3:A:402:BTB:O1	3:A:402:BTB:H52	2.18	0.43
1:B:51:GLU:C	1:B:53:LEU:H	2.22	0.43
1:C:50:LEU:O	1:C:53:LEU:HB2	2.19	0.43
1:D:43:LEU:HD13	1:E:-2:PHE:HE2	1.83	0.43
1:E:164:LEU:HD23	1:E:164:LEU:HA	1.88	0.43
1:A:123:VAL:N	1:A:124:PRO:HD2	2.33	0.43
1:B:136:LEU:HA	1:B:136:LEU:HD23	1.75	0.43
1:B:299:ILE:HD12	1:B:302:ARG:NH2	2.34	0.43
1:D:61:ASP:OD2	1:D:66:TYR:OH	2.35	0.43
1:B:40:SER:OG	1:B:72:ASP:OD2	2.22	0.42
1:B:205:LEU:HD12	1:B:209:ALA:HB2	2.00	0.42
1:F:44:THR:HB	1:F:65:ARG:HB3	2.01	0.42
1:C:-1:GLN:O	1:C:0:SER:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:TYR:HE2	1:C:172:ILE:CD1	2.27	0.42
1:D:351:ASN:OD1	1:D:351:ASN:C	2.57	0.42
1:E:57:LYS:HB2	1:E:57:LYS:HE3	1.78	0.42
1:E:162:PHE:O	1:E:163:GLU:C	2.58	0.42
1:A:115:ASP:O	1:A:361:VAL:HA	2.19	0.42
1:B:165:GLY:O	1:B:169:LEU:HB2	2.19	0.42
3:E:402:BTB:H62	3:E:402:BTB:H71	1.65	0.42
1:B:26:TYR:HA	1:B:285:ALA:HB1	2.02	0.42
1:C:206:LEU:HD23	1:C:206:LEU:HA	1.77	0.42
1:C:337:ARG:HD2	1:C:338:PHE:CZ	2.54	0.42
1:D:157:LYS:CD	1:E:-3:TYR:CE1	3.03	0.42
1:C:21:TRP:CD1	1:C:272:ILE:HG23	2.54	0.42
1:D:157:LYS:HE3	1:D:157:LYS:CA	2.49	0.42
1:F:317:GLY:HA2	2:F:401:HIR:CHA	2.50	0.42
1:B:147:TRP:O	1:B:151:VAL:HG23	2.20	0.42
1:B:239:LEU:HD22	1:B:301:ASP:HB3	2.02	0.42
1:C:-10:HIS:CG	1:C:-9:HIS:N	2.87	0.42
1:C:157:LYS:HE3	1:C:157:LYS:HA	2.01	0.42
1:C:210:GLY:HA3	2:C:401:HIR:CMC	2.49	0.42
1:D:223:ILE:HD11	1:D:360:LEU:HD13	2.01	0.42
1:E:21:TRP:CD1	1:E:272:ILE:HG23	2.54	0.42
1:D:26:TYR:HA	1:D:285:ALA:HB1	2.01	0.42
1:F:110:ILE:O	1:F:112:PRO:HD3	2.18	0.42
1:B:160:GLU:O	1:B:163:GLU:HG3	2.19	0.42
1:C:121:LEU:C	1:C:124:PRO:HD2	2.40	0.42
1:D:46:TYR:CE1	1:D:66:TYR:HB3	2.54	0.42
1:E:160:GLU:HB3	1:E:162:PHE:CD2	2.54	0.42
1:F:49:ARG:HH21	1:F:58:ILE:HD13	1.85	0.42
1:A:150:LEU:O	1:A:154:ARG:HG2	2.20	0.42
1:A:160:GLU:O	1:A:163:GLU:HG3	2.20	0.42
1:A:175:VAL:O	1:A:179:LEU:HG	2.20	0.42
1:B:117:ILE:HD12	1:B:117:ILE:HG23	1.64	0.42
1:B:117:ILE:HD13	1:B:117:ILE:HA	1.67	0.42
1:D:277:TYR:CD2	1:E:-4:LEU:HD13	2.54	0.42
1:F:-7:HIS:O	1:F:-6:GLU:HB2	2.20	0.42
1:F:150:LEU:HD13	1:F:167:LYS:HB2	2.01	0.42
1:F:351:ASN:HD21	1:F:353:VAL:CG1	2.32	0.42
1:B:98:PHE:CE2	1:B:132:LYS:HG2	2.55	0.42
1:B:205:LEU:HD12	1:B:209:ALA:CB	2.50	0.42
1:B:217:LEU:HD22	1:B:248:LEU:HD21	2.01	0.42
1:C:86:ILE:HG23	1:C:87:PHE:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:ARG:HD3	1:D:284:SER:OG	2.20	0.42
1:E:160:GLU:HB3	1:E:162:PHE:HD2	1.85	0.42
1:F:38:LYS:HG2	1:F:263:GLU:OE2	2.19	0.42
1:F:40:SER:HB2	1:F:262:LYS:HG3	2.02	0.42
1:C:148:SER:HA	1:C:208:ILE:CG2	2.50	0.41
1:B:235:ARG:HE	1:B:339:ARG:NH1	2.18	0.41
1:C:-10:HIS:ND1	1:C:-9:HIS:N	2.68	0.41
1:E:338:PHE:CE2	1:E:364:LEU:HD13	2.55	0.41
1:F:226:THR:HG21	1:F:343:ILE:HG13	2.01	0.41
1:A:-7:HIS:O	1:A:-6:GLU:HB2	2.19	0.41
1:A:351:ASN:OD1	1:A:353:VAL:N	2.42	0.41
1:B:-2:PHE:HE2	1:C:43:LEU:HD13	1.83	0.41
1:B:95:LEU:CD1	1:B:133:ILE:HD11	2.51	0.41
1:B:123:VAL:HG11	1:B:145:LYS:HE2	2.02	0.41
1:C:118:VAL:HG23	1:C:360:LEU:HB3	2.03	0.41
1:D:175:VAL:O	1:D:179:LEU:HD12	2.19	0.41
3:D:402:BTB:O1	3:D:402:BTB:C5	2.68	0.41
1:B:150:LEU:HD21	1:B:168:TYR:HB2	2.03	0.41
1:E:157:LYS:HD3	1:F:-3:TYR:CE1	2.55	0.41
1:A:-10:HIS:CE1	1:C:-8:HIS:CD2	3.08	0.41
1:A:150:LEU:CG	1:A:164:LEU:HD13	2.50	0.41
1:B:162:PHE:O	1:B:163:GLU:C	2.59	0.41
1:C:136:LEU:HD23	1:C:136:LEU:HA	1.84	0.41
1:C:157:LYS:HE3	1:C:157:LYS:CA	2.50	0.41
3:C:402:BTB:O4	3:C:402:BTB:H81	2.20	0.41
1:E:150:LEU:HD11	1:E:164:LEU:HD13	2.01	0.41
1:A:210:GLY:HA3	2:A:401:HIR:C2C	2.50	0.41
1:C:162:PHE:O	1:C:163:GLU:C	2.58	0.41
1:E:43:LEU:HD13	1:F:-2:PHE:CE2	2.55	0.41
1:F:9:ARG:O	1:F:13:PRO:HG3	2.21	0.41
1:B:353:VAL:HG13	1:B:354:LEU:HG	2.02	0.41
1:C:90:GLN:O	1:C:94:THR:HG23	2.21	0.41
1:C:168:TYR:CE2	1:C:172:ILE:HD12	2.54	0.41
1:E:30:LYS:HG2	1:E:34:ASN:ND2	2.36	0.41
1:F:123:VAL:N	1:F:124:PRO:HD2	2.36	0.41
1:F:205:LEU:HD21	2:F:401:HIR:CMD	2.51	0.41
1:A:-1:GLN:O	1:A:3:ASP:HB2	2.21	0.41
1:A:142:GLU:CG	1:A:145:LYS:HE3	2.51	0.41
1:B:194:LEU:HD23	1:B:198:GLU:HB3	2.02	0.41
1:C:17:ASP:OD1	1:C:17:ASP:C	2.58	0.41
1:C:223:ILE:HG13	1:C:357:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:VAL:HG12	1:C:259:ARG:N	2.36	0.41
1:D:328:ARG:HD3	1:D:332:GLU:OE2	2.20	0.41
1:E:223:ILE:HD11	1:E:360:LEU:CD1	2.51	0.41
1:F:136:LEU:HD23	1:F:136:LEU:HA	1.85	0.41
3:C:402:BTB:H62	3:C:402:BTB:H71	1.83	0.41
1:E:194:LEU:HB3	1:E:198:GLU:HB2	2.03	0.40
1:B:123:VAL:H	1:B:124:PRO:HD2	1.86	0.40
1:B:134:LEU:C	1:B:183:THR:HG23	2.42	0.40
1:C:53:LEU:HD23	1:C:53:LEU:HA	1.76	0.40
1:C:164:LEU:HD23	1:C:164:LEU:HA	1.94	0.40
1:D:351:ASN:HD21	1:D:353:VAL:CG1	2.34	0.40
1:E:344:LEU:HD11	1:E:363:ARG:HB2	2.03	0.40
1:F:164:LEU:HD23	1:F:164:LEU:HA	1.99	0.40
1:B:351:ASN:OD1	1:B:352:GLU:N	2.55	0.40
1:D:61:ASP:OD1	1:D:65:ARG:NH1	2.54	0.40
1:D:95:LEU:HD11	1:D:133:ILE:HG12	2.03	0.40
1:E:301:ASP:OD1	1:E:301:ASP:N	2.54	0.40
1:F:51:GLU:C	1:F:53:LEU:N	2.73	0.40
1:F:57:LYS:HB2	1:F:57:LYS:HE3	1.77	0.40
1:F:344:LEU:HD11	1:F:363:ARG:HB2	2.03	0.40
1:A:99:ILE:HG21	1:A:329:ILE:HD12	2.03	0.40
1:B:246:GLU:HG3	1:B:298:PHE:CE2	2.57	0.40
1:E:175:VAL:O	1:E:179:LEU:HD13	2.22	0.40
1:A:36:PHE:CE2	1:A:73:PRO:HG2	2.57	0.40
1:C:99:ILE:HG12	1:C:129:VAL:CG2	2.51	0.40
1:D:-10:HIS:CE1	1:E:-10:HIS:CE1	3.08	0.40
1:D:43:LEU:HB3	1:E:-2:PHE:CD2	2.57	0.40
1:D:165:GLY:HA2	1:D:169:LEU:HG	2.04	0.40
1:D:256:ARG:HD3	1:D:281:TRP:CZ3	2.56	0.40
1:E:194:LEU:HD22	1:E:198:GLU:OE2	2.21	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	377/385 (98%)	348 (92%)	23 (6%)	6 (2%)	9	40
1	B	377/385 (98%)	347 (92%)	24 (6%)	6 (2%)	9	40
1	C	377/385 (98%)	348 (92%)	24 (6%)	5 (1%)	12	44
1	D	377/385 (98%)	348 (92%)	23 (6%)	6 (2%)	9	40
1	E	377/385 (98%)	347 (92%)	23 (6%)	7 (2%)	8	36
1	F	377/385 (98%)	347 (92%)	25 (7%)	5 (1%)	12	44
All	All	2262/2310 (98%)	2085 (92%)	142 (6%)	35 (2%)	10	41

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-8	HIS
1	A	-6	GLU
1	A	57	LYS
1	A	163	GLU
1	B	-6	GLU
1	B	57	LYS
1	C	-6	GLU
1	C	57	LYS
1	D	-6	GLU
1	D	57	LYS
1	E	-6	GLU
1	F	-6	GLU
1	F	57	LYS
1	F	163	GLU
1	B	163	GLU
1	C	163	GLU
1	D	-9	HIS
1	D	163	GLU
1	E	-9	HIS
1	E	57	LYS
1	E	163	GLU
1	A	155	TRP
1	B	155	TRP
1	C	155	TRP
1	D	155	TRP
1	E	155	TRP
1	F	155	TRP

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Mol	Chain	Res	Type
1	A	182	GLY
1	C	182	GLY
1	F	182	GLY
1	B	182	GLY
1	B	317	GLY
1	E	182	GLY
1	E	317	GLY
1	D	317	GLY

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	347/353 (98%)	337 (97%)	10 (3%)	42	72
1	B	347/353 (98%)	339 (98%)	8 (2%)	50	76
1	C	347/353 (98%)	339 (98%)	8 (2%)	50	76
1	D	347/353 (98%)	339 (98%)	8 (2%)	50	76
1	E	347/353 (98%)	340 (98%)	7 (2%)	55	79
1	F	347/353 (98%)	341 (98%)	6 (2%)	60	82
All	All	2082/2118 (98%)	2035 (98%)	47 (2%)	50	76

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-10	HIS
1	A	-7	HIS
1	A	-4	LEU
1	A	0	SER
1	A	59	ARG
1	A	90	GLN
1	A	162	PHE
1	A	287	ARG
1	A	339	ARG
1	A	351	ASN

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Mol	Chain	Res	Type
1	B	-10	HIS
1	B	-9	HIS
1	B	-4	LEU
1	B	0	SER
1	B	59	ARG
1	B	162	PHE
1	B	168	TYR
1	B	287	ARG
1	C	-10	HIS
1	C	-9	HIS
1	C	-4	LEU
1	C	0	SER
1	C	59	ARG
1	C	202	TYR
1	C	287	ARG
1	C	351	ASN
1	D	-11	HIS
1	D	-9	HIS
1	D	-4	LEU
1	D	0	SER
1	D	59	ARG
1	D	287	ARG
1	D	316	LEU
1	D	351	ASN
1	E	-9	HIS
1	E	-7	HIS
1	E	-4	LEU
1	E	0	SER
1	E	59	ARG
1	E	287	ARG
1	E	351	ASN
1	F	-10	HIS
1	F	-4	LEU
1	F	0	SER
1	F	59	ARG
1	F	98	PHE
1	F	287	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN

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Mol	Chain	Res	Type
1	A	191	ASN
1	B	35	ASN
1	E	35	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	BTB	A	402	-	13,13,13	1.65	3 (23%)	7,16,16	1.44	1 (14%)
3	BTB	B	402	-	13,13,13	1.78	2 (15%)	7,16,16	1.79	2 (28%)
2	HIR	D	401	-	42,52,52	1.20	4 (9%)	45,87,87	1.50	6 (13%)
2	HIR	E	401	-	42,52,52	1.27	6 (14%)	45,87,87	1.36	4 (8%)
2	HIR	C	401	-	42,52,52	1.18	6 (14%)	45,87,87	1.45	8 (17%)
3	BTB	F	402	-	13,13,13	1.48	2 (15%)	7,16,16	1.26	1 (14%)
2	HIR	F	401	-	42,52,52	1.39	6 (14%)	45,87,87	1.38	5 (11%)
2	HIR	B	401	-	42,52,52	1.36	7 (16%)	45,87,87	1.66	8 (17%)
3	BTB	D	402	-	13,13,13	1.66	3 (23%)	7,16,16	1.72	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BTB	C	402	-	13,13,13	1.32	2 (15%)	7,16,16	1.45	2 (28%)
2	HIR	A	401	-	42,52,52	1.31	5 (11%)	45,87,87	1.54	9 (20%)
3	BTB	E	402	-	13,13,13	1.59	3 (23%)	7,16,16	1.41	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BTB	A	402	-	-	6/21/21/21	-
3	BTB	B	402	-	-	7/21/21/21	-
2	HIR	D	401	-	1/1/3/10	2/14/66/66	-
2	HIR	E	401	-	1/1/3/10	3/14/66/66	-
2	HIR	C	401	-	1/1/3/10	3/14/66/66	-
3	BTB	F	402	-	-	7/21/21/21	-
2	HIR	F	401	-	1/1/3/10	1/14/66/66	-
2	HIR	B	401	-	1/1/3/10	2/14/66/66	-
3	BTB	D	402	-	-	10/21/21/21	-
3	BTB	C	402	-	-	7/21/21/21	-
2	HIR	A	401	-	1/1/3/10	2/14/66/66	-
3	BTB	E	402	-	-	6/21/21/21	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	BTB	C3-C2	4.72	1.59	1.53
3	A	402	BTB	C3-C2	4.13	1.59	1.53
3	E	402	BTB	C3-C2	3.83	1.58	1.53
3	D	402	BTB	C3-C2	3.68	1.58	1.53
3	F	402	BTB	C3-C2	3.47	1.58	1.53
3	D	402	BTB	C4-C2	3.37	1.57	1.53
3	C	402	BTB	C3-C2	3.25	1.57	1.53
2	F	401	HIR	CAB-C3B	3.20	1.56	1.47
2	B	401	HIR	CMB-C2B	3.11	1.57	1.50
3	B	402	BTB	C4-C2	3.04	1.57	1.53
2	B	401	HIR	CAA-C2A	3.00	1.56	1.52
3	F	402	BTB	C4-C2	2.84	1.57	1.53
2	E	401	HIR	CAC-C3C	2.82	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	HIR	CAB-C3B	2.79	1.55	1.47
2	C	401	HIR	CAC-C3C	2.77	1.55	1.47
2	B	401	HIR	CMD-C2D	2.65	1.56	1.50
3	A	402	BTB	C4-C2	2.64	1.57	1.53
3	E	402	BTB	C4-C2	2.63	1.56	1.53
2	C	401	HIR	CMC-C2C	2.54	1.56	1.50
2	A	401	HIR	CMD-C2D	2.53	1.56	1.50
2	E	401	HIR	CMC-C2C	2.53	1.56	1.50
2	F	401	HIR	C4B-NB	-2.51	1.34	1.38
2	F	401	HIR	CMD-C2D	2.50	1.56	1.50
2	D	401	HIR	CMC-C2C	2.43	1.55	1.50
2	C	401	HIR	CAB-C3B	2.42	1.54	1.47
2	F	401	HIR	CAC-C3C	2.38	1.53	1.47
3	E	402	BTB	C2-N	2.37	1.53	1.48
2	D	401	HIR	CAC-C3C	2.35	1.53	1.47
2	B	401	HIR	CAC-C3C	2.34	1.53	1.47
2	A	401	HIR	CMC-C2C	2.30	1.55	1.50
2	B	401	HIR	CMC-C2C	2.29	1.55	1.50
2	C	401	HIR	CMD-C2D	2.29	1.55	1.50
2	E	401	HIR	C3C-C2C	-2.29	1.32	1.37
3	C	402	BTB	C4-C2	2.26	1.56	1.53
2	D	401	HIR	CMB-C2B	2.26	1.55	1.50
2	F	401	HIR	CMC-C2C	2.20	1.55	1.50
2	A	401	HIR	CAA-C2A	2.20	1.55	1.52
2	A	401	HIR	CHB-C1B	2.19	1.40	1.35
2	A	401	HIR	CAC-C3C	2.16	1.53	1.47
3	A	402	BTB	C2-N	2.13	1.52	1.48
2	E	401	HIR	CMB-C2B	2.12	1.55	1.50
2	D	401	HIR	CAB-C3B	2.11	1.53	1.47
2	C	401	HIR	O1A-CGA	2.08	1.29	1.22
2	F	401	HIR	CHC-C4B	-2.08	1.34	1.39
2	B	401	HIR	CAB-C3B	2.07	1.53	1.47
2	C	401	HIR	CMB-C2B	2.06	1.55	1.50
2	B	401	HIR	C3C-C2C	-2.06	1.33	1.37
3	D	402	BTB	C2-N	2.04	1.52	1.48
2	E	401	HIR	C2A-C3A	-2.04	1.31	1.37

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	HIR	CBA-CAA-C2A	-5.10	103.92	112.62
2	E	401	HIR	CAD-CBD-CGD	-5.03	102.78	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	HIR	CBA-CAA-C2A	-4.97	104.14	112.62
2	A	401	HIR	C4C-C3C-C2C	4.10	110.12	106.75
2	D	401	HIR	C4B-C3B-C2B	3.64	110.01	107.11
2	A	401	HIR	C4B-C3B-C2B	3.60	109.98	107.11
2	C	401	HIR	C4B-C3B-C2B	3.56	109.94	107.11
2	B	401	HIR	C4B-C3B-C2B	3.49	109.89	107.11
2	B	401	HIR	CAD-CBD-CGD	-3.47	106.14	113.60
3	D	402	BTB	O4-C4-C2	3.39	120.73	111.44
2	F	401	HIR	C4C-C3C-C2C	3.32	109.48	106.75
3	B	402	BTB	O3-C3-C2	3.31	120.50	111.44
2	B	401	HIR	C4C-C3C-C2C	3.16	109.35	106.75
2	E	401	HIR	CBA-CAA-C2A	-3.12	107.30	112.62
2	A	401	HIR	CAD-CBD-CGD	-3.11	106.90	113.60
2	C	401	HIR	CAA-CBA-CGA	-3.08	105.12	113.76
3	A	402	BTB	O3-C3-C2	3.02	119.72	111.44
2	F	401	HIR	CMA-C3A-C4A	-2.93	123.96	128.46
2	D	401	HIR	C4C-C3C-C2C	2.83	109.08	106.75
2	C	401	HIR	C4C-C3C-C2C	2.82	109.07	106.75
2	F	401	HIR	CHD-C4C-C3C	2.79	130.02	125.26
2	C	401	HIR	CBA-CAA-C2A	-2.67	108.07	112.62
3	D	402	BTB	O3-C3-C2	2.62	118.61	111.44
2	E	401	HIR	C4B-C3B-C2B	2.62	109.19	107.11
3	B	402	BTB	O4-C4-C2	2.59	118.52	111.44
2	A	401	HIR	C4A-C3A-C2A	2.57	108.78	107.00
2	B	401	HIR	C4A-C3A-C2A	2.52	108.75	107.00
2	A	401	HIR	O1A-CGA-CBA	-2.49	115.07	123.08
3	E	402	BTB	O3-C3-C2	2.48	118.22	111.44
2	E	401	HIR	CMC-C2C-C1C	2.44	129.02	124.71
3	C	402	BTB	O4-C4-C2	2.32	117.80	111.44
3	F	402	BTB	O3-C3-C2	2.31	117.76	111.44
2	C	401	HIR	CAD-C3D-C2D	-2.30	123.59	127.88
2	A	401	HIR	CBC-CAC-C3C	-2.28	116.28	127.62
2	F	401	HIR	CAC-C3C-C2C	-2.27	121.14	128.60
2	A	401	HIR	O2A-CGA-CBA	2.22	121.18	114.03
2	B	401	HIR	CMB-C2B-C1B	2.20	128.38	125.04
2	A	401	HIR	CMC-C2C-C1C	2.18	128.55	124.71
2	B	401	HIR	CHD-C4C-C3C	2.17	128.97	125.26
2	D	401	HIR	CBC-CAC-C3C	-2.17	116.82	127.62
2	D	401	HIR	O2D-CGD-CBD	-2.16	116.13	123.08
2	A	401	HIR	CAA-CBA-CGA	-2.16	107.72	113.76
2	C	401	HIR	O1A-CGA-CBA	-2.10	116.35	123.08
2	C	401	HIR	CBB-CAB-C3B	-2.08	117.28	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	HIR	O1A-CGA-CBA	-2.05	116.48	123.08
2	D	401	HIR	C4D-ND-C1D	2.05	109.18	107.01
2	C	401	HIR	CAD-C3D-C4D	2.05	128.24	124.66
3	C	402	BTB	O3-C3-C2	2.02	116.97	111.44
2	F	401	HIR	C4D-ND-C1D	2.02	109.14	107.01

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	401	HIR	NC
2	B	401	HIR	NC
2	C	401	HIR	NC
2	D	401	HIR	NC
2	E	401	HIR	NC
2	F	401	HIR	NC

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	HIR	C2C-C3C-CAC-CBC
2	C	401	HIR	C4C-C3C-CAC-CBC
3	A	402	BTB	C1-C2-C4-O4
3	A	402	BTB	C3-C2-C4-O4
3	A	402	BTB	C6-C5-N-C7
3	A	402	BTB	N-C5-C6-O6
3	B	402	BTB	C1-C2-C4-O4
3	B	402	BTB	C3-C2-C4-O4
3	B	402	BTB	N-C2-C4-O4
3	B	402	BTB	C6-C5-N-C7
3	C	402	BTB	C1-C2-C4-O4
3	C	402	BTB	C3-C2-C4-O4
3	C	402	BTB	N-C2-C4-O4
3	C	402	BTB	C6-C5-N-C7
3	D	402	BTB	C1-C2-C4-O4
3	D	402	BTB	C3-C2-C4-O4
3	D	402	BTB	N-C2-C4-O4
3	D	402	BTB	C4-C2-N-C7
3	D	402	BTB	N-C5-C6-O6
3	E	402	BTB	C1-C2-C4-O4
3	E	402	BTB	C3-C2-C4-O4
3	E	402	BTB	N-C2-C4-O4
3	E	402	BTB	C6-C5-N-C7

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Mol	Chain	Res	Type	Atoms
3	E	402	BTB	N-C5-C6-O6
3	F	402	BTB	C1-C2-C4-O4
3	F	402	BTB	C3-C2-C4-O4
3	F	402	BTB	N-C2-C4-O4
3	F	402	BTB	C6-C5-N-C7
3	B	402	BTB	N-C5-C6-O6
3	C	402	BTB	N-C5-C6-O6
3	F	402	BTB	N-C5-C6-O6
3	A	402	BTB	N-C7-C8-O8
3	D	402	BTB	N-C7-C8-O8
3	E	402	BTB	N-C7-C8-O8
3	F	402	BTB	N-C7-C8-O8
3	B	402	BTB	N-C7-C8-O8
2	A	401	HIR	C2C-C3C-CAC-CBC
2	B	401	HIR	C2C-C3C-CAC-CBC
2	D	401	HIR	C2C-C3C-CAC-CBC
2	E	401	HIR	C2C-C3C-CAC-CBC
3	C	402	BTB	N-C7-C8-O8
2	A	401	HIR	C4C-C3C-CAC-CBC
2	B	401	HIR	C4C-C3C-CAC-CBC
2	D	401	HIR	C4C-C3C-CAC-CBC
2	E	401	HIR	C4C-C3C-CAC-CBC
3	D	402	BTB	C6-C5-N-C7
3	A	402	BTB	N-C2-C4-O4
3	B	402	BTB	C4-C2-N-C7
3	C	402	BTB	C4-C2-N-C7
3	D	402	BTB	N-C2-C3-O3
3	D	402	BTB	C1-C2-N-C7
3	F	402	BTB	C4-C2-N-C7
2	F	401	HIR	C4C-C3C-CAC-CBC
3	D	402	BTB	C1-C2-C3-O3
2	E	401	HIR	CAD-CBD-CGD-O1D
2	C	401	HIR	CAD-CBD-CGD-O1D

There are no ring outliers.

12 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	BTB	2	0
3	B	402	BTB	2	0
2	D	401	HIR	1	0
2	E	401	HIR	2	0

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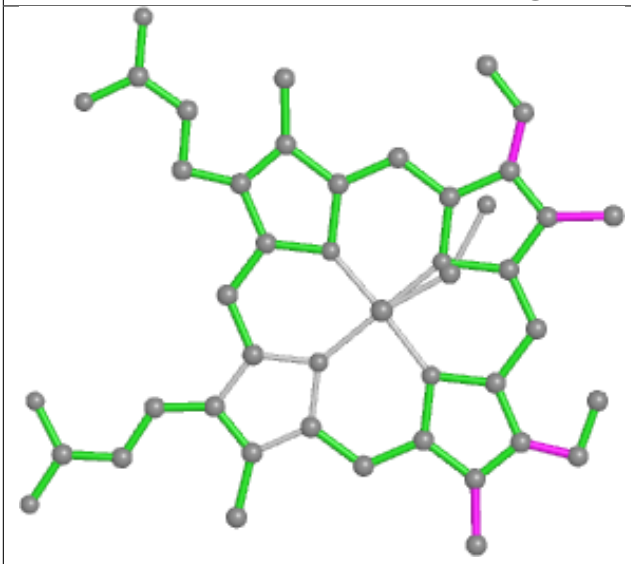
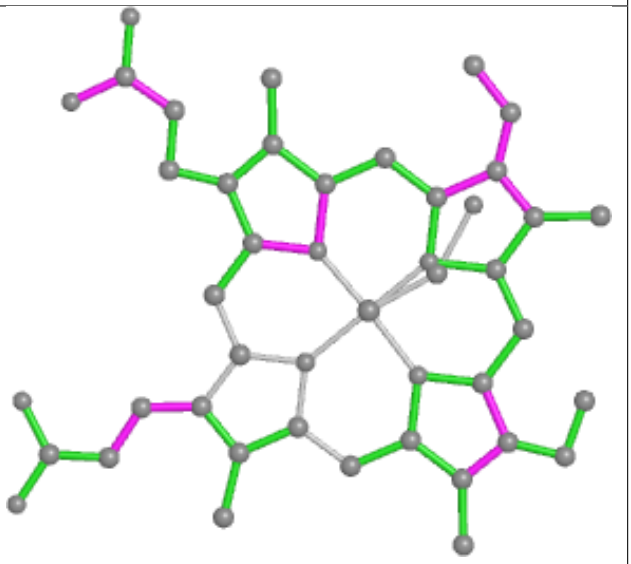
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	HIR	4	0
3	F	402	BTB	2	0
2	F	401	HIR	3	0
2	B	401	HIR	2	0
3	D	402	BTB	2	0
3	C	402	BTB	3	0
2	A	401	HIR	2	0
3	E	402	BTB	1	0

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.

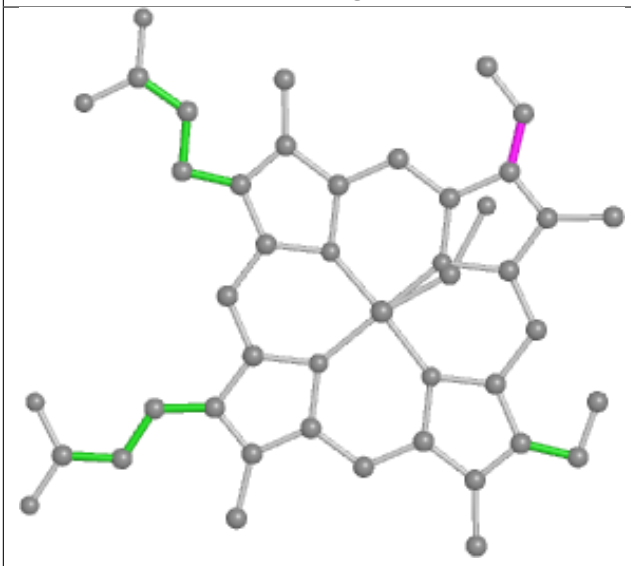
Ligand HIR D 401



Bond lengths



Bond angles



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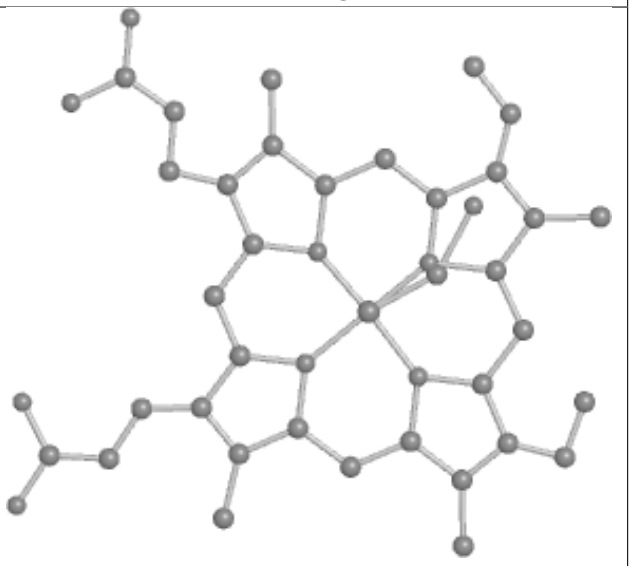
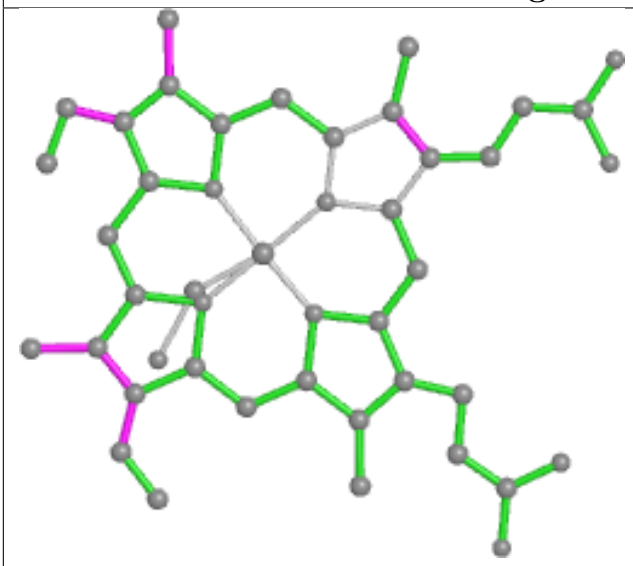
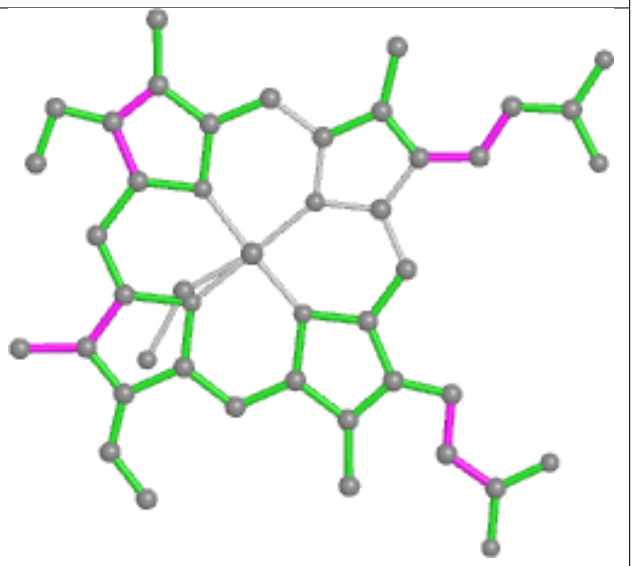


Rings

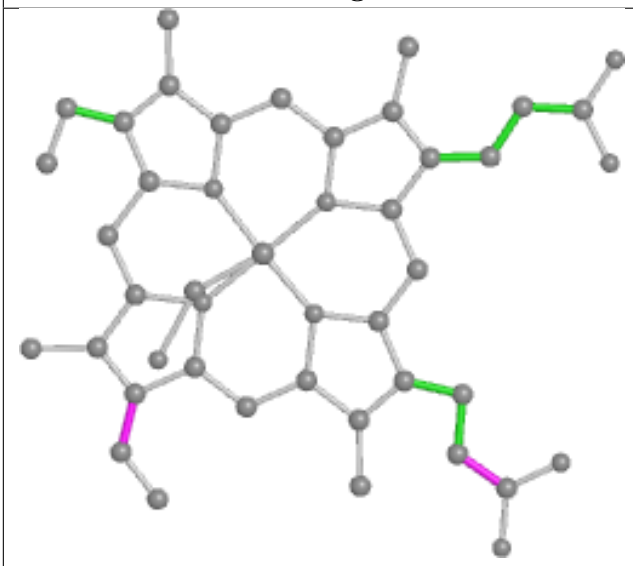
Ligand HIR E 401



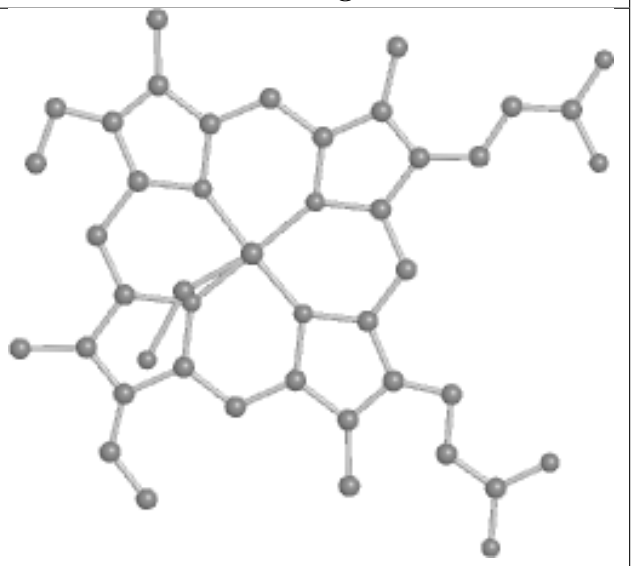
Bond lengths



Bond angles

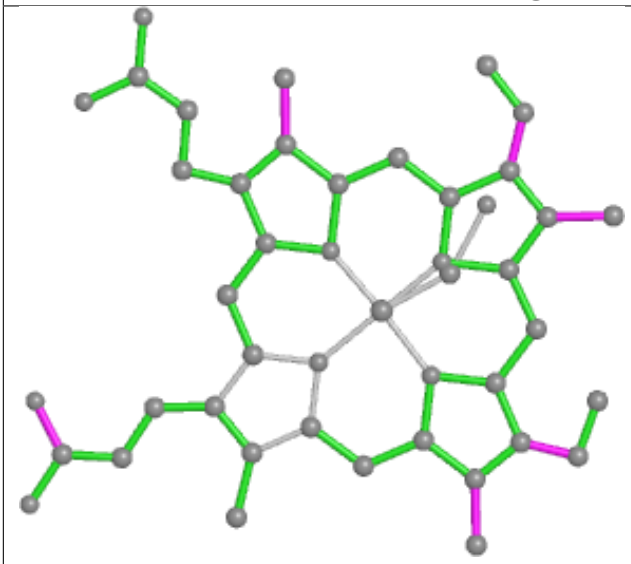


Torsions

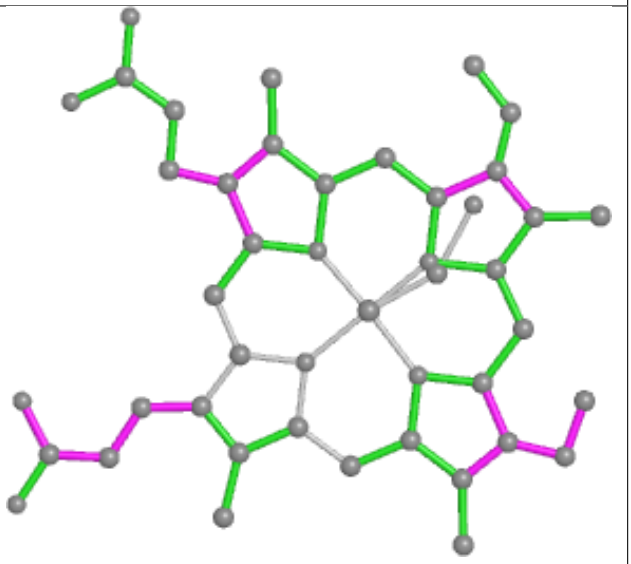


Rings

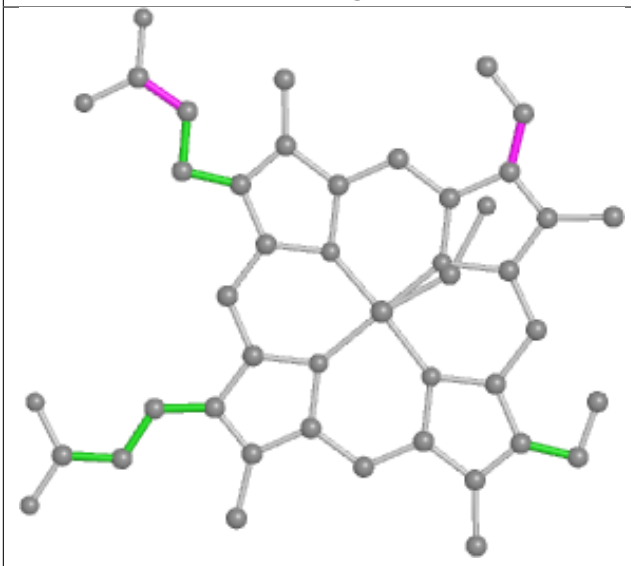
Ligand HIR C 401



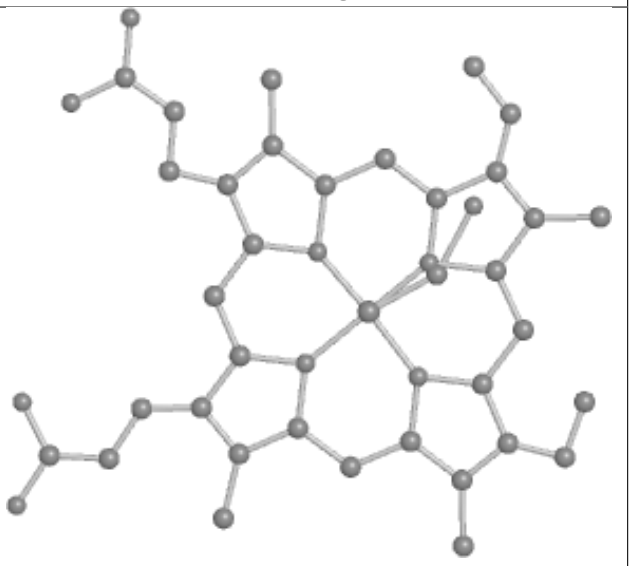
Bond lengths



Bond angles

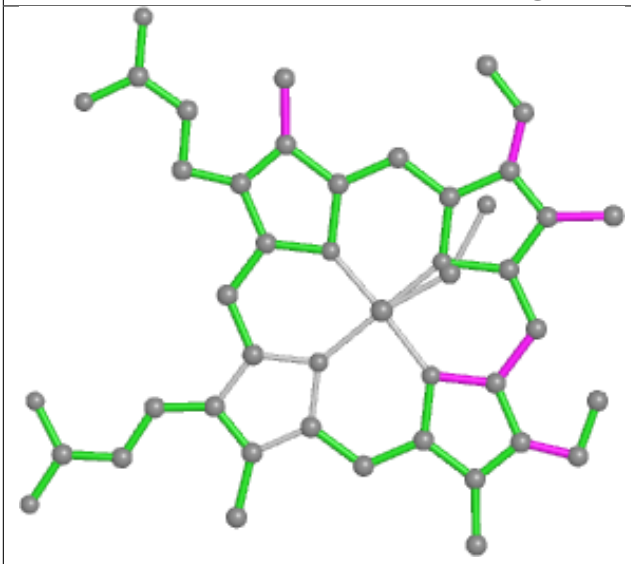


Torsions

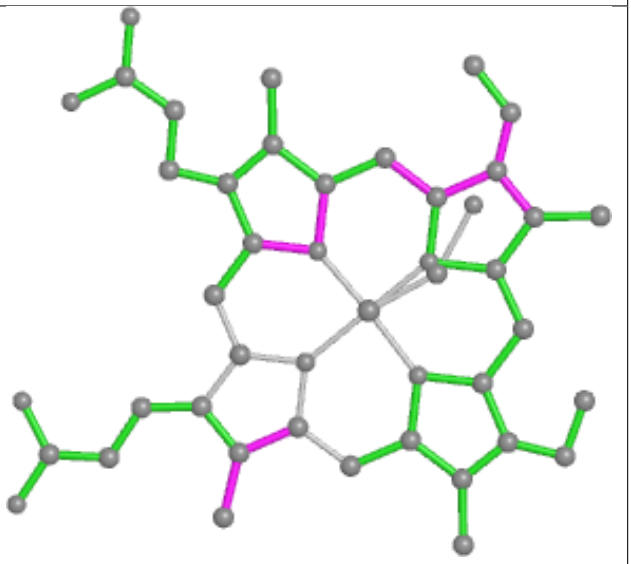


Rings

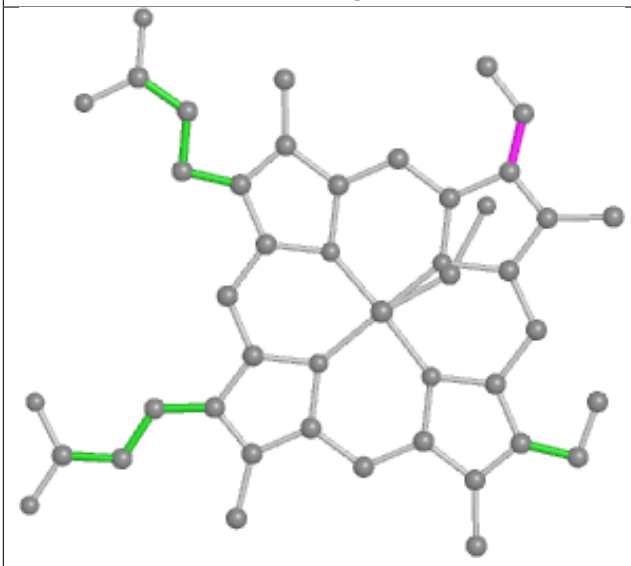
Ligand HIR F 401



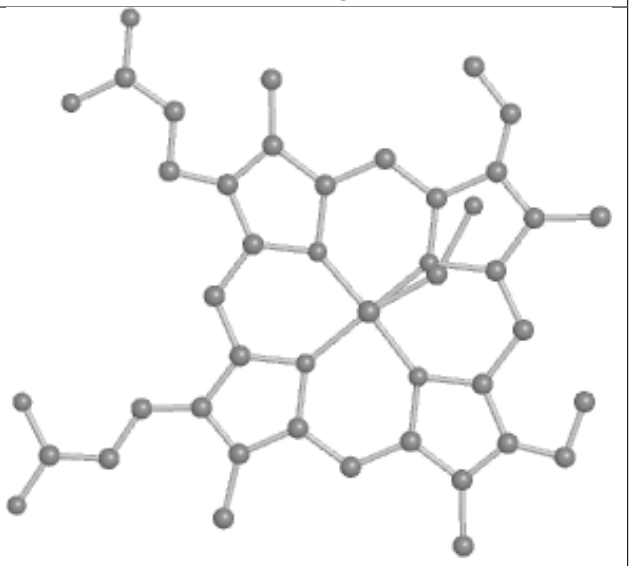
Bond lengths



Bond angles

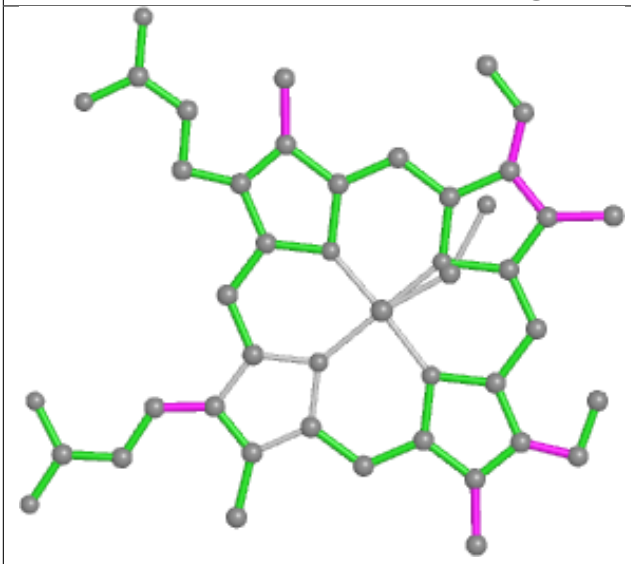


Torsions

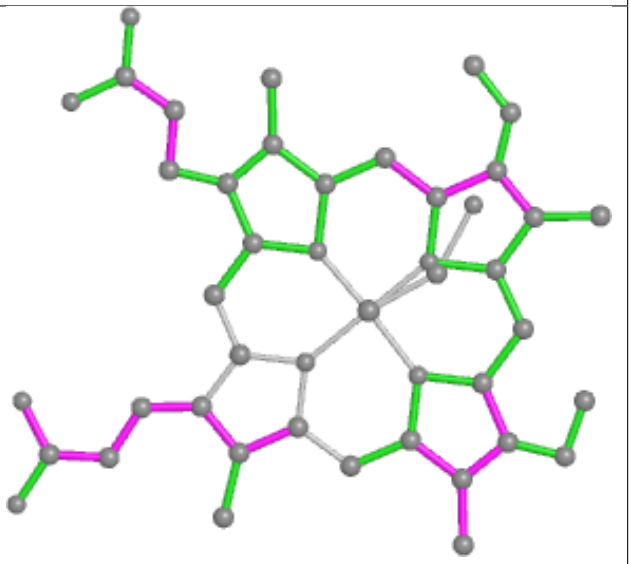


Rings

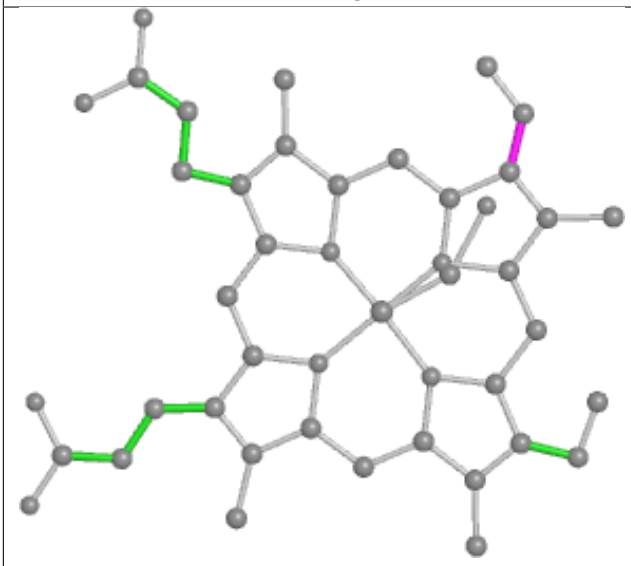
Ligand HIR B 401



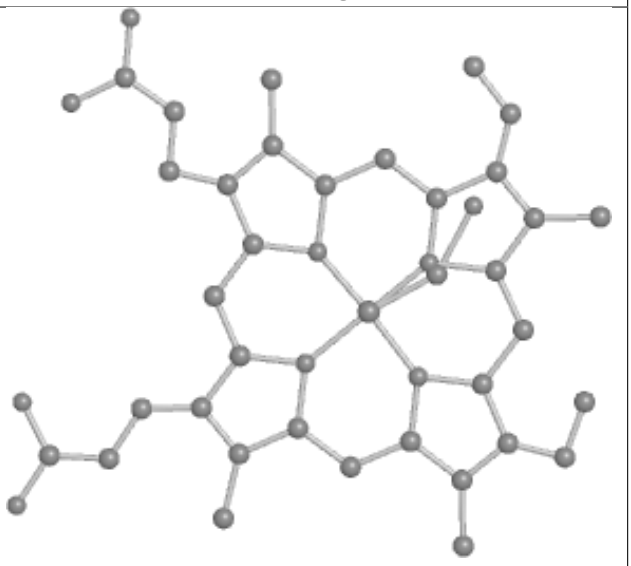
Bond lengths



Bond angles

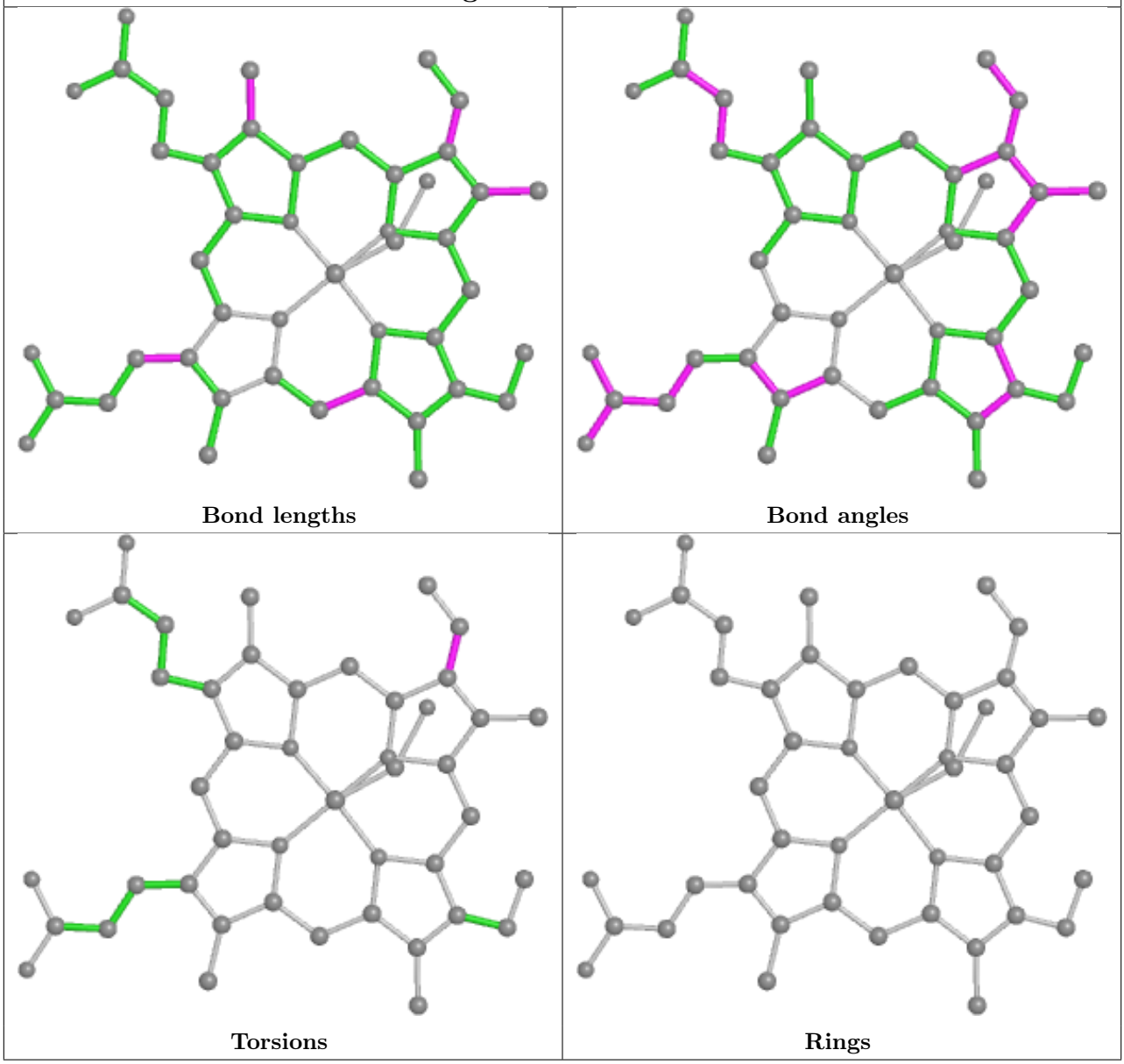


Torsions



Rings

Ligand HIR A 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	379/385 (98%)	0.08	5 (1%)	77	66	36, 72, 148, 205	0
1	B	379/385 (98%)	0.11	9 (2%)	59	43	38, 76, 151, 197	0
1	C	379/385 (98%)	0.24	4 (1%)	80	70	37, 77, 143, 193	0
1	D	379/385 (98%)	0.10	6 (1%)	72	59	42, 80, 148, 201	0
1	E	379/385 (98%)	0.17	9 (2%)	59	43	43, 83, 158, 207	0
1	F	379/385 (98%)	0.33	8 (2%)	63	49	42, 101, 172, 210	0
All	All	2274/2310 (98%)	0.17	41 (1%)	68	55	36, 81, 154, 210	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	367	ASN	9.0
1	B	367	ASN	6.2
1	B	61	ASP	3.9
1	E	366	SER	3.6
1	E	62	ILE	3.0
1	E	162	PHE	2.9
1	F	43	LEU	2.8
1	E	161	ILE	2.8
1	E	160	GLU	2.7
1	A	164	LEU	2.7
1	B	366	SER	2.6
1	E	338	PHE	2.5
1	F	352	GLU	2.5
1	E	164	LEU	2.5
1	B	62	ILE	2.5
1	D	60	PHE	2.4
1	B	189	VAL	2.4
1	D	162	PHE	2.4
1	A	163	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	338	PHE	2.3
1	F	338	PHE	2.3
1	F	62	ILE	2.3
1	D	367	ASN	2.3
1	C	164	LEU	2.3
1	D	203	ILE	2.2
1	A	158	PRO	2.2
1	B	161	ILE	2.2
1	C	352	GLU	2.2
1	A	159	GLY	2.2
1	F	331	ILE	2.1
1	A	367	ASN	2.1
1	F	61	ASP	2.1
1	D	164	LEU	2.1
1	B	338	PHE	2.1
1	C	43	LEU	2.1
1	E	189	VAL	2.1
1	B	164	LEU	2.0
1	F	254	LEU	2.0
1	B	-2	PHE	2.0
1	F	-2	PHE	2.0
1	C	69	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 monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BTB	B	402	14/14	0.83	0.35	53,110,140,145	0

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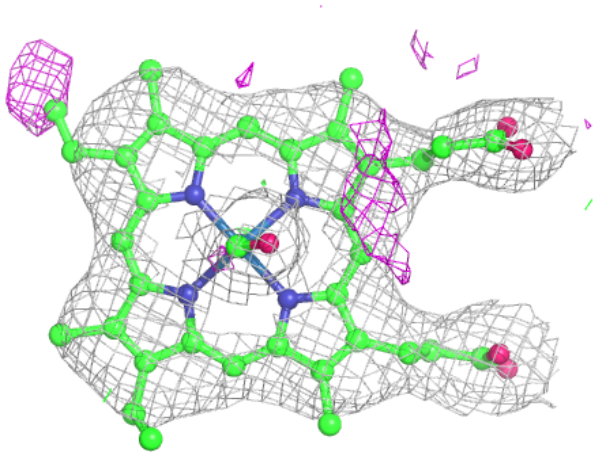
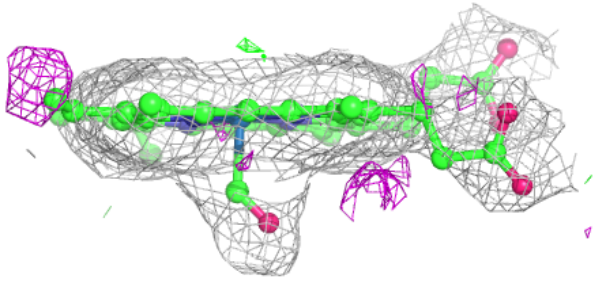
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BTB	D	402	14/14	0.83	0.36	59,110,139,152	0
3	BTB	F	402	14/14	0.83	0.50	52,113,139,147	0
3	BTB	A	402	14/14	0.85	0.32	45,99,125,138	0
3	BTB	E	402	14/14	0.88	0.45	56,96,133,150	0
3	BTB	C	402	14/14	0.88	0.43	50,109,143,147	0
2	HIR	A	401	45/45	0.99	0.28	33,58,66,66	0
2	HIR	B	401	45/45	0.99	0.29	42,52,69,73	0
2	HIR	C	401	45/45	0.99	0.33	23,64,74,77	0
2	HIR	D	401	45/45	0.99	0.28	25,59,74,80	0
2	HIR	E	401	45/45	0.99	0.30	42,66,82,89	0
2	HIR	F	401	45/45	0.99	0.30	54,69,79,81	0
4	NI	A	403	1/1	1.00	0.23	45,45,45,45	0
4	NI	D	403	1/1	1.00	0.20	48,48,48,48	0

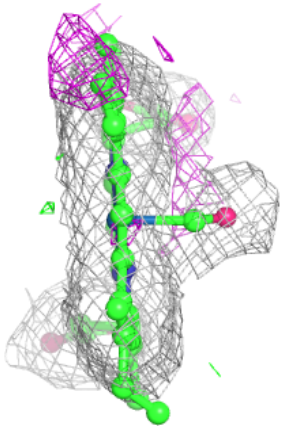
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HIR A 401:

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

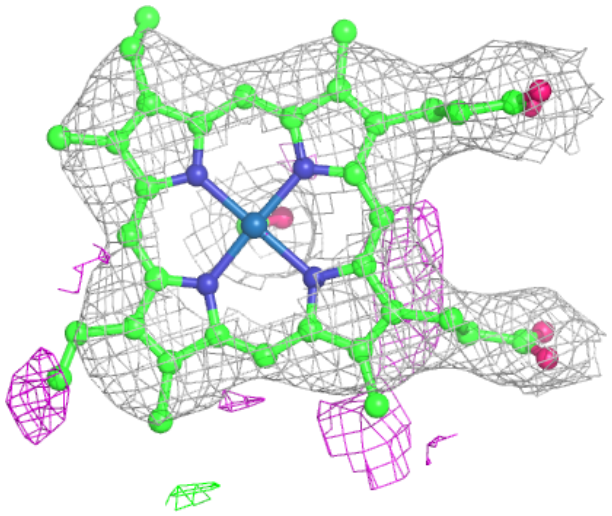


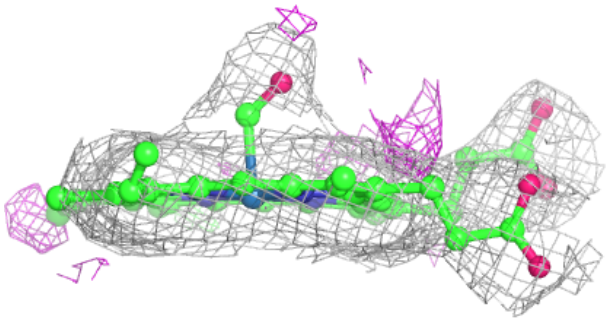


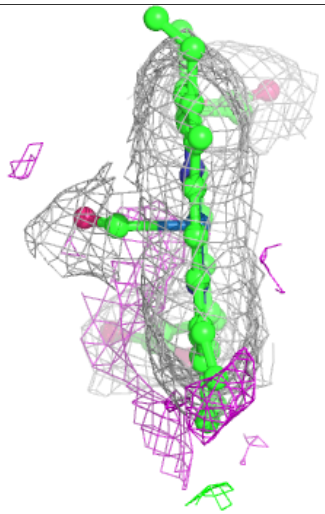


Electron density around HIR B 401:

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

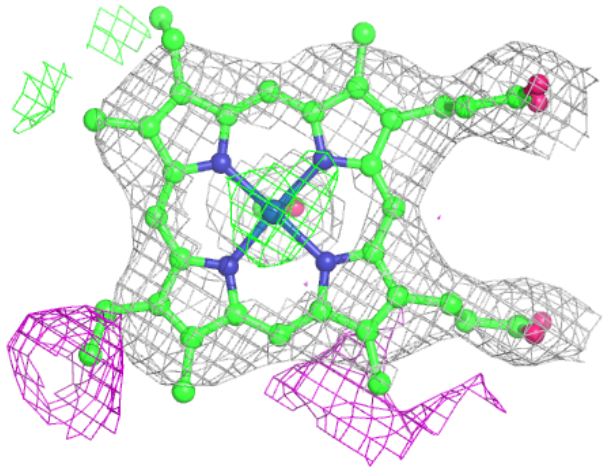


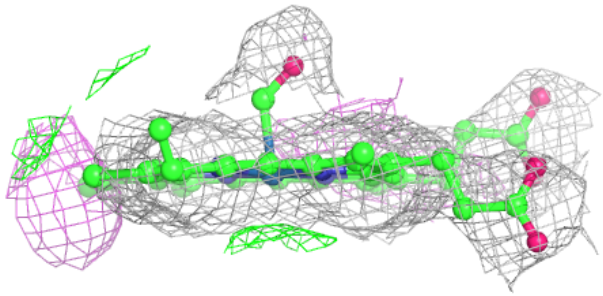




Electron density around HIR C 401:

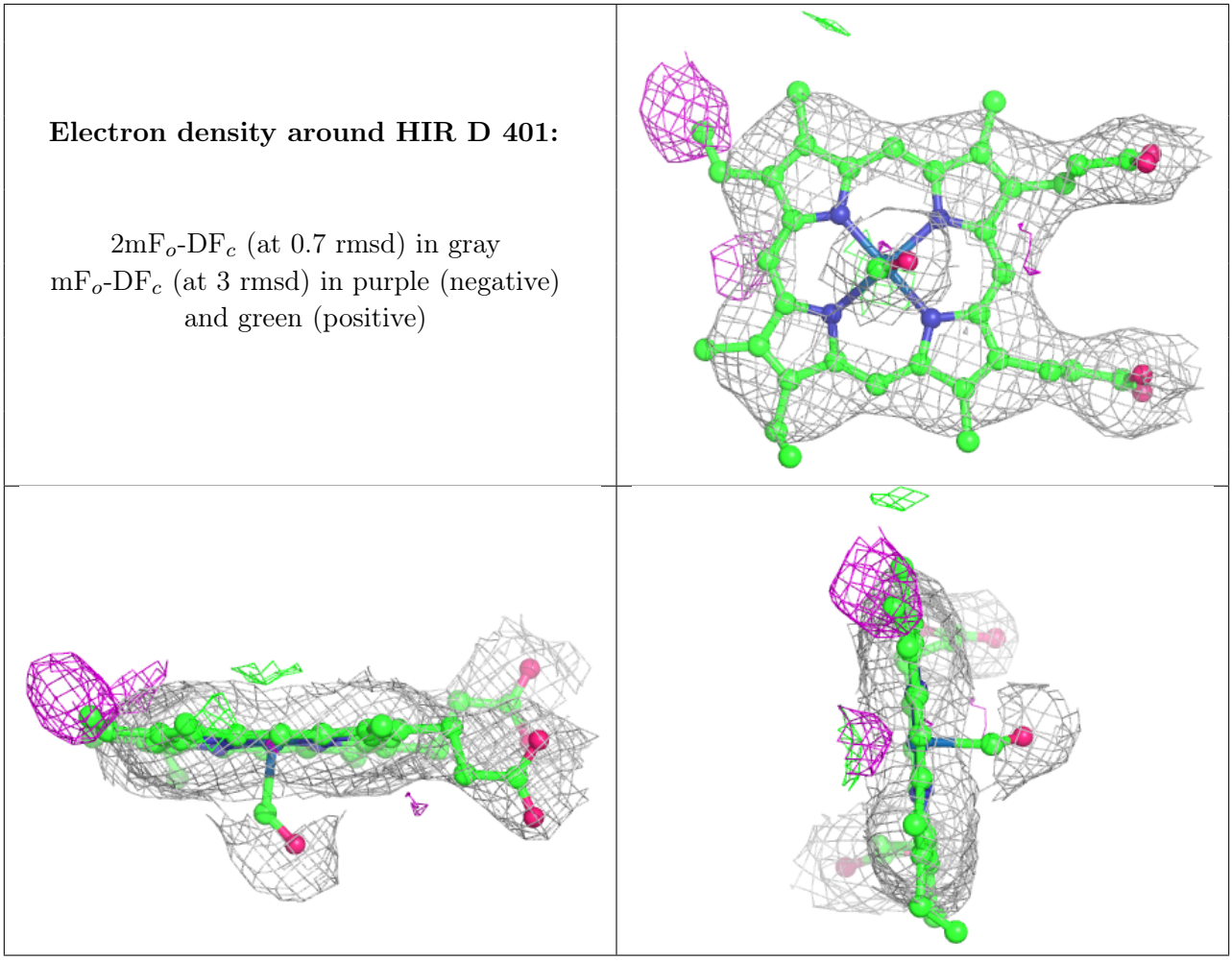
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





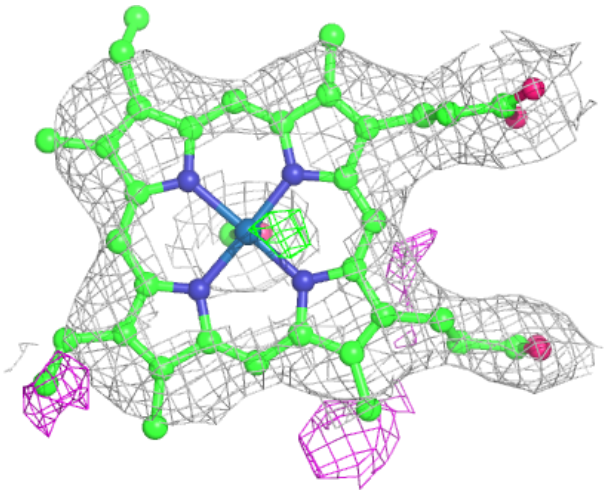
Electron density around HIR D 401:

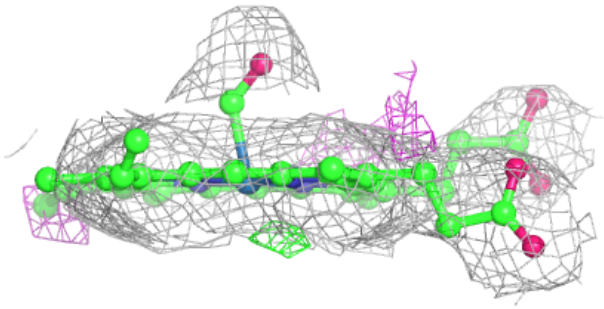
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

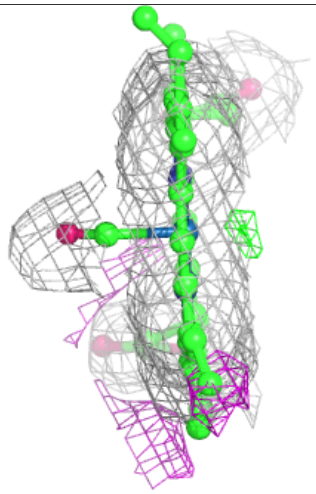


Electron density around HIR E 401:

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

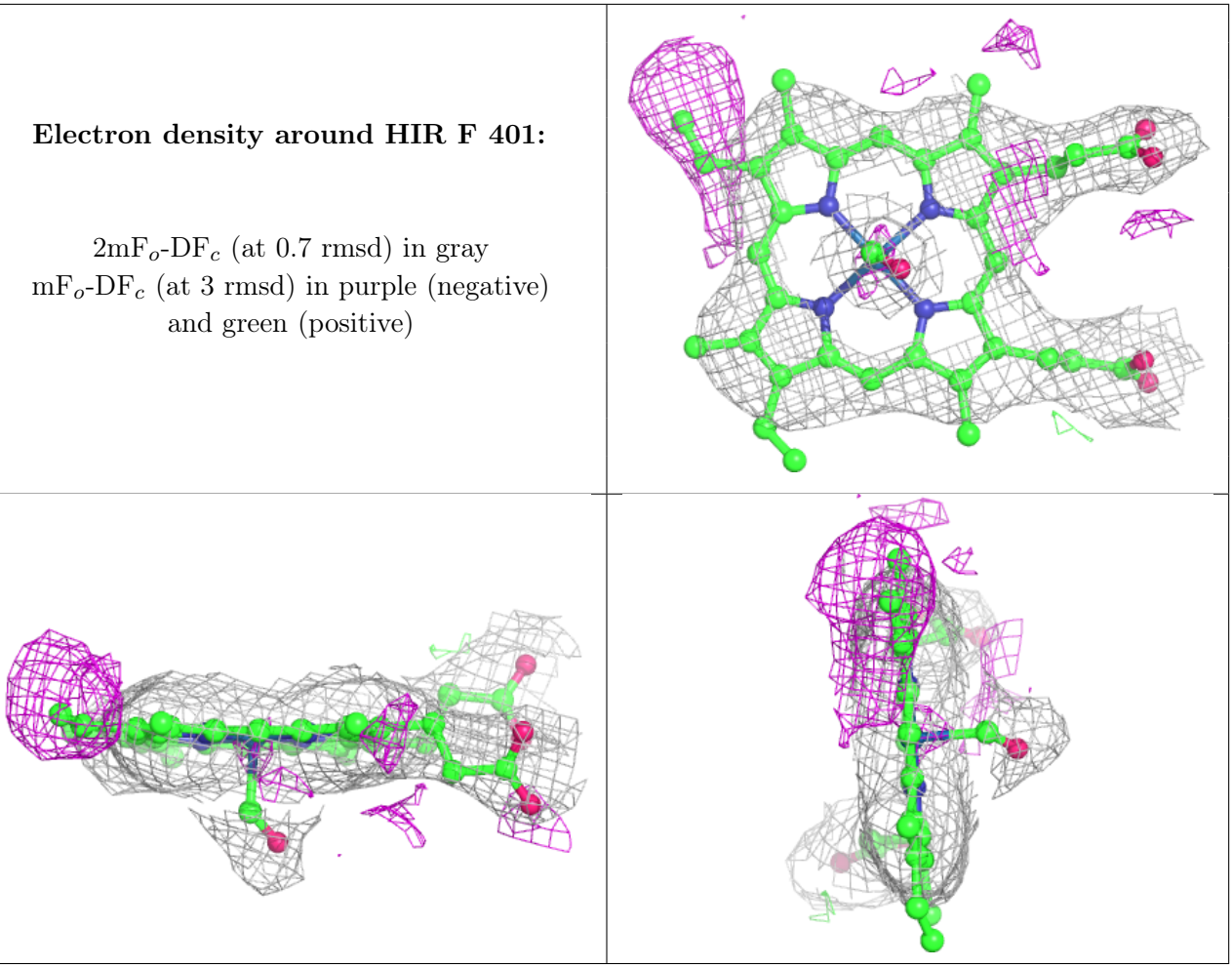






Electron density around HIR F 401:

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



6.5 Other polymers

There are no such residues in this entry.