



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:35 am BST

PDB ID : 3L4D
Title : Crystal structure of sterol 14-alpha demethylase (CYP51) from Leishmania infantum in complex with fluconazole
Authors : Lepesheva, G.I.; Hargrove, T.Y.; Wawrzak, Z.; Waterman, M.R.
Deposited on : 2009-12-19
Resolution : 2.75 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 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 : 2.11
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) : 2.11

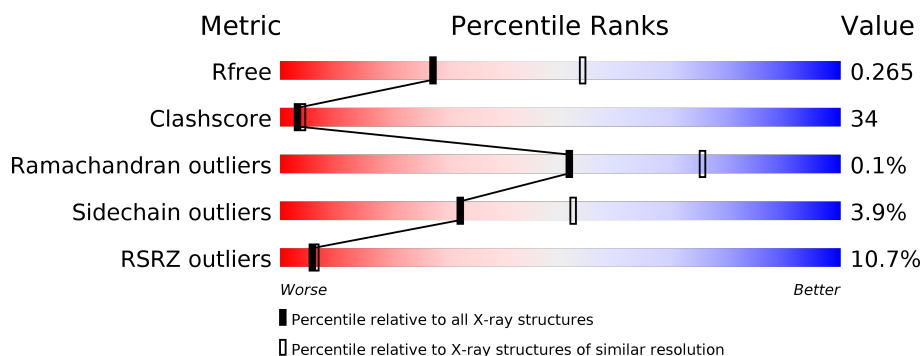
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	453	<div> <div>8%</div> <div>56%</div> <div>40%</div> <div>..</div> </div>
1	B	453	<div> <div>9%</div> <div>59%</div> <div>36%</div> <div>..</div> </div>
1	C	453	<div> <div>13%</div> <div>50%</div> <div>46%</div> <div>..</div> </div>
1	D	453	<div> <div>12%</div> <div>51%</div> <div>44%</div> <div>..</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14534 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.

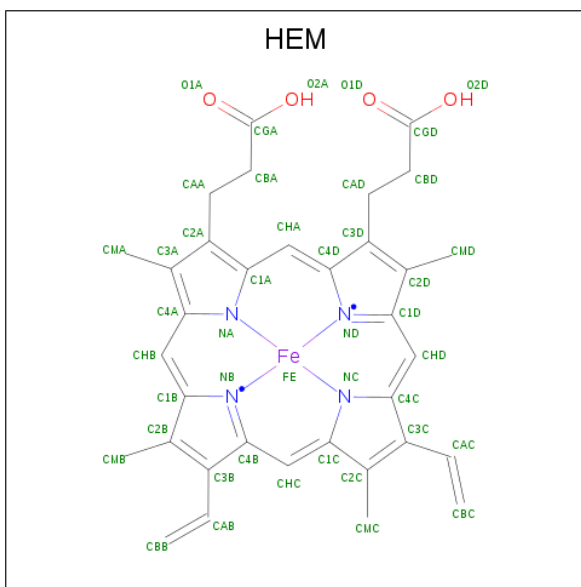
- Molecule 1 is a protein called Sterol 14-alpha demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3553	2270	619	635	29			
1	B	449	Total	C	N	O	S	0	0	0
			3562	2276	621	636	29			
1	C	447	Total	C	N	O	S	0	0	0
			3545	2266	617	633	29			
1	D	445	Total	C	N	O	S	0	0	0
			3529	2257	615	628	29			

There are 16 discrepancies between the modelled and reference sequences:

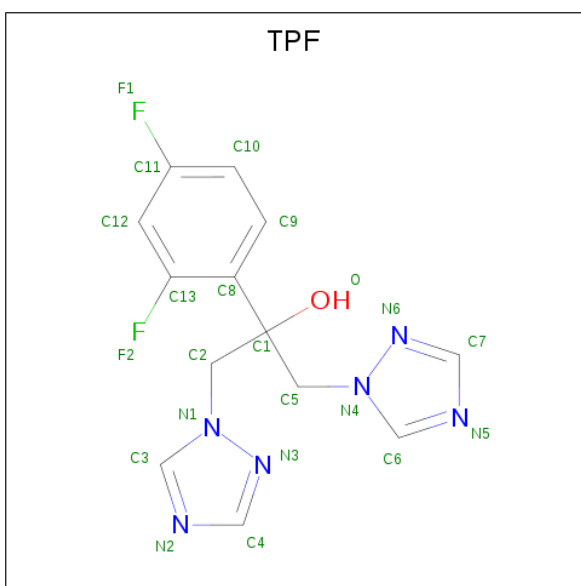
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	LYS	-	EXPRESSION TAG	UNP A2TEF2
A	29	GLY	-	EXPRESSION TAG	UNP A2TEF2
A	30	LYS	-	EXPRESSION TAG	UNP A2TEF2
A	31	LEU	-	EXPRESSION TAG	UNP A2TEF2
B	28	LYS	-	EXPRESSION TAG	UNP A2TEF2
B	29	GLY	-	EXPRESSION TAG	UNP A2TEF2
B	30	LYS	-	EXPRESSION TAG	UNP A2TEF2
B	31	LEU	-	EXPRESSION TAG	UNP A2TEF2
C	28	LYS	-	EXPRESSION TAG	UNP A2TEF2
C	29	GLY	-	EXPRESSION TAG	UNP A2TEF2
C	30	LYS	-	EXPRESSION TAG	UNP A2TEF2
C	31	LEU	-	EXPRESSION TAG	UNP A2TEF2
D	28	LYS	-	EXPRESSION TAG	UNP A2TEF2
D	29	GLY	-	EXPRESSION TAG	UNP A2TEF2
D	30	LYS	-	EXPRESSION TAG	UNP A2TEF2
D	31	LEU	-	EXPRESSION TAG	UNP A2TEF2

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



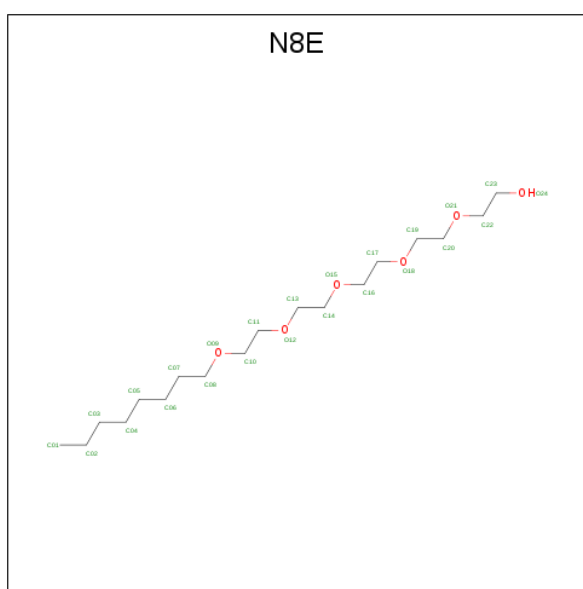
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 2-(2,4-DIFLUOROPHENYL)-1,3-DI(1H-1,2,4-TRIAZOL-1-YL)PROPAN-2-OL (three-letter code: TPF) (formula: $C_{13}H_{12}F_2N_6O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			22	13	2	6	1		
3	B	1	Total	C	F	N	O	0	0
			22	13	2	6	1		
3	C	1	Total	C	F	N	O	0	0
			22	13	2	6	1		
3	D	1	Total	C	F	N	O	0	0
			22	13	2	6	1		

- Molecule 4 is 3,6,9,12,15-PENTAOXATRICOSAN-1-OL (three-letter code: N8E) (formula: $C_{18}H_{38}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			24	18	6		

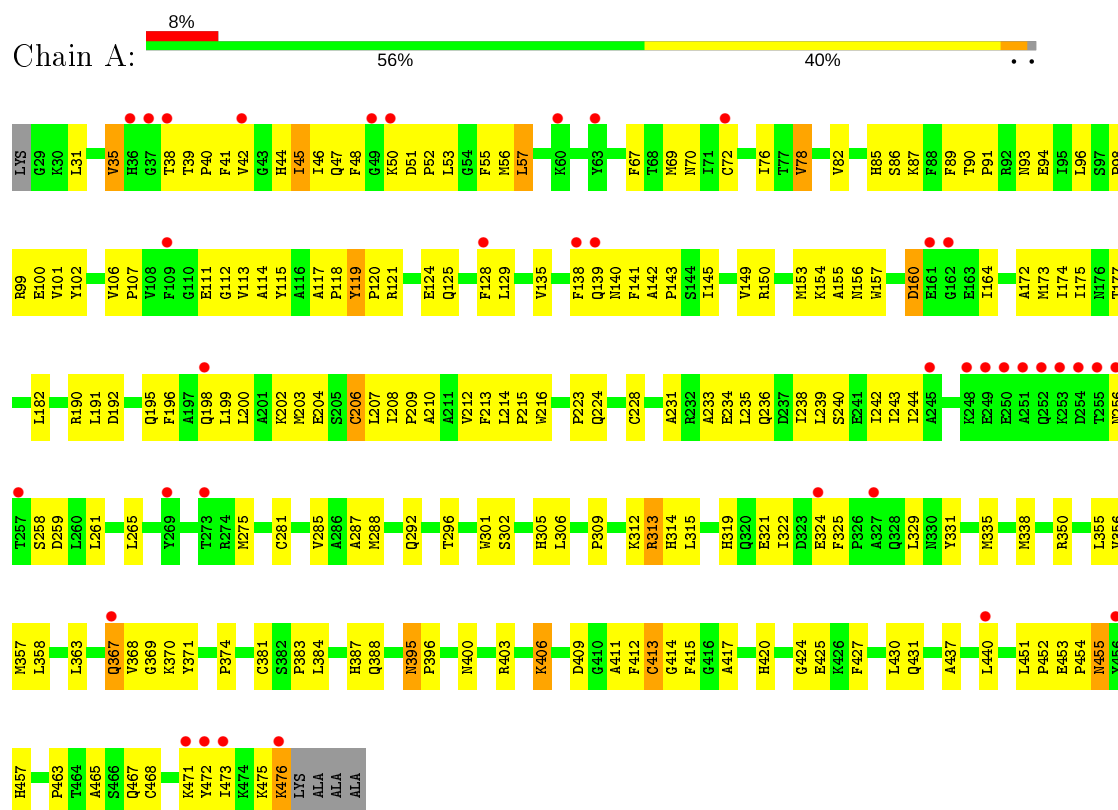
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	16	Total	O	0	0
			16	16		
5	B	11	Total	O	0	0
			11	11		
5	C	16	Total	O	0	0
			16	16		
5	D	18	Total	O	0	0
			18	18		

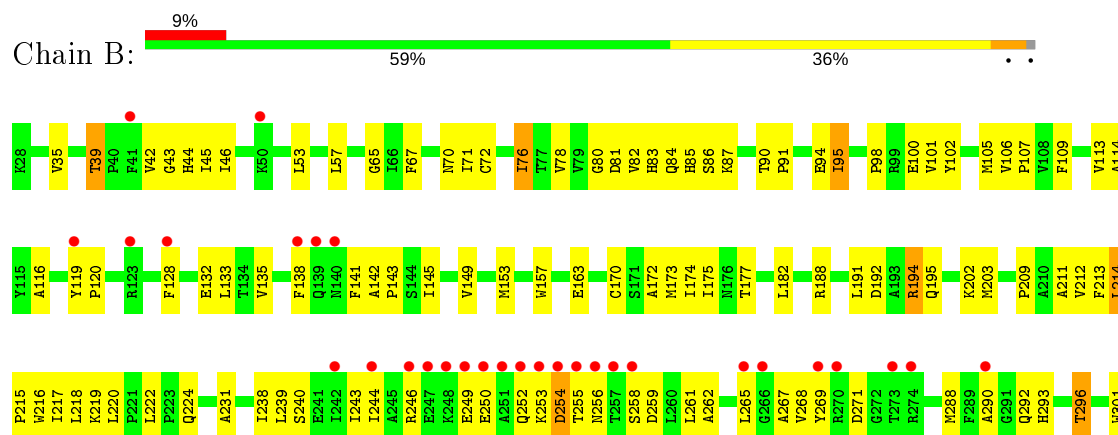
3 Residue-property plots [i](#)

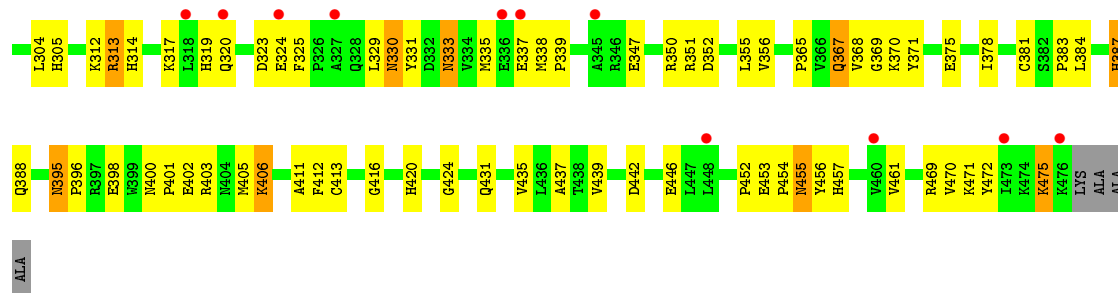
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Sterol 14-alpha demethylase

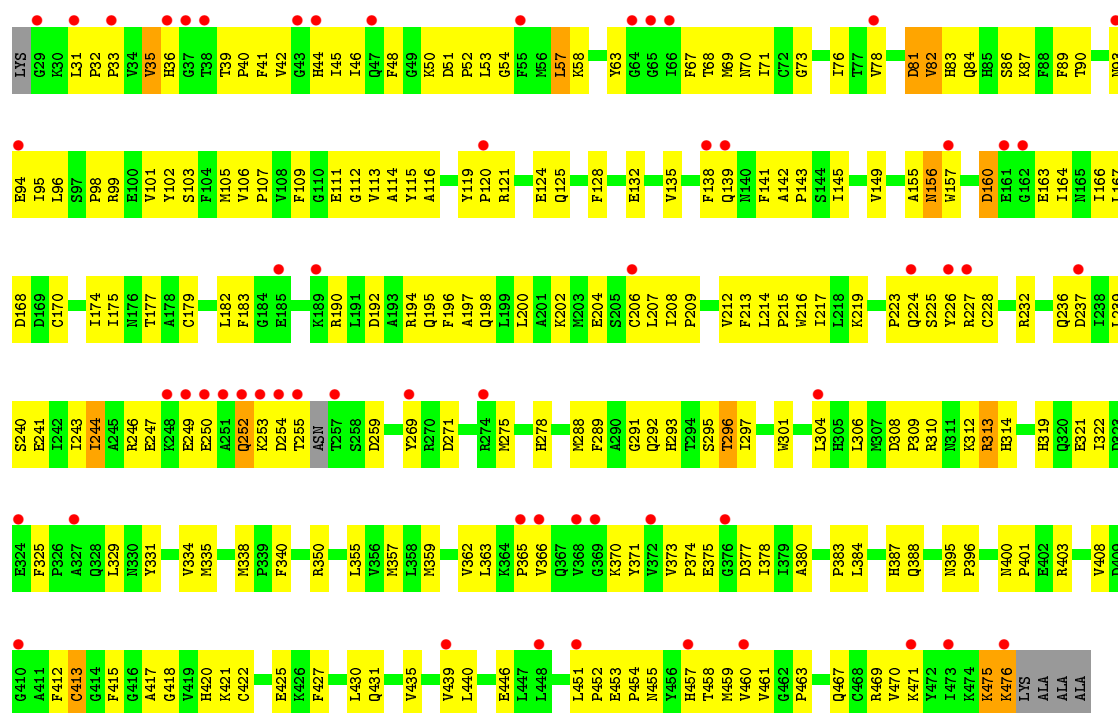


• Molecule 1: Sterol 14-alpha demethylase

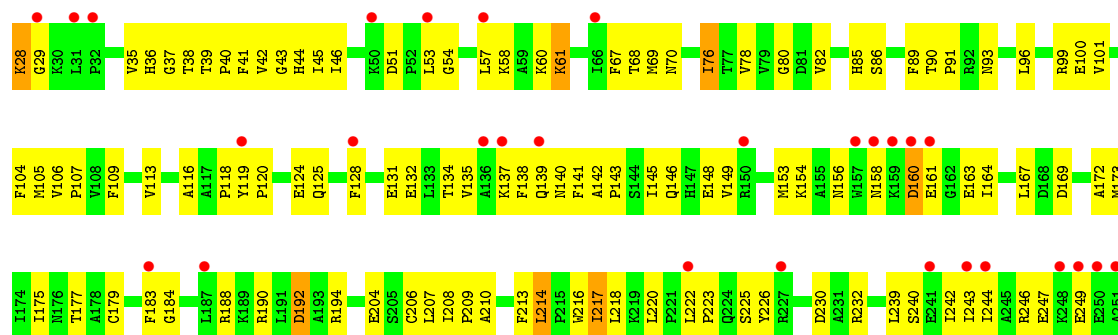


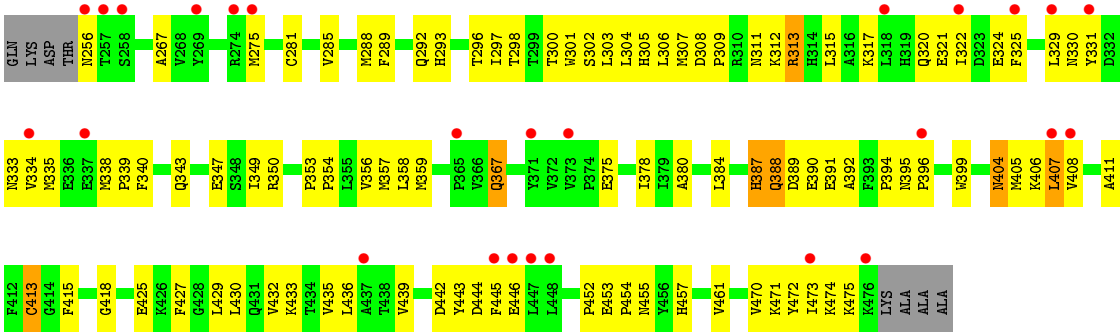


• Molecule 1: Sterol 14-alpha demethylase



• Molecule 1: Sterol 14-alpha demethylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.89Å 118.51Å 100.96Å 90.00° 104.82° 90.00°	Depositor
Resolution (Å)	48.80 – 2.75 48.80 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.80-2.75) 97.6 (48.80-2.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.219 , 0.267 0.216 , 0.265	Depositor DCC
R_{free} test set	2495 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	90.4	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 76.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14534	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: N8E, TPF, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/3636	0.44	0/4917
1	B	0.27	0/3645	0.41	0/4928
1	C	0.37	1/3627 (0.0%)	0.42	0/4903
1	D	0.32	0/3611	0.39	0/4881
All	All	0.35	1/14519 (0.0%)	0.42	0/19629

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	413	CYS	CB-SG	-5.28	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3553	0	3579	246	0
1	B	3562	0	3592	201	0
1	C	3545	0	3572	287	0
1	D	3529	0	3559	262	0
2	A	43	0	30	6	0
2	B	43	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	43	0	30	8	0
2	D	43	0	30	8	0
3	A	22	0	12	6	0
3	B	22	0	12	6	0
3	C	22	0	12	6	0
3	D	22	0	12	4	0
4	C	24	0	38	8	0
5	A	16	0	0	0	0
5	B	11	0	0	0	0
5	C	16	0	0	1	0
5	D	18	0	0	2	0
All	All	14534	0	14508	982	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 34.

All (982) 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:D:213:PHE:C	1:D:214:LEU:HD22	1.48	1.32
1:C:252:GLN:NE2	1:C:254:ASP:HB3	1.48	1.29
1:A:209:PRO:O	1:A:212:VAL:HG23	1.35	1.25
1:D:407:LEU:O	1:D:407:LEU:HD12	1.38	1.18
1:B:292:GLN:O	1:B:296:THR:HG22	1.43	1.17
1:A:292:GLN:O	1:A:296:THR:HG23	1.48	1.14
1:D:388:GLN:HE21	1:D:388:GLN:CA	1.61	1.13
1:C:292:GLN:O	1:C:296:THR:HG23	1.50	1.12
1:D:367:GLN:HE21	1:D:367:GLN:N	1.49	1.11
1:B:330:ASN:N	1:B:333:ASN:HD21	1.47	1.10
1:D:388:GLN:HE21	1:D:388:GLN:N	1.51	1.09
1:D:334:VAL:HA	1:D:338:MET:SD	1.94	1.07
1:A:206:CYS:HB3	1:A:228:CYS:SG	1.95	1.07
1:D:288:MET:HE2	1:D:288:MET:HA	1.34	1.07
1:D:407:LEU:C	1:D:407:LEU:HD12	1.78	1.02
1:B:330:ASN:H	1:B:333:ASN:ND2	1.57	1.02
1:C:44:HIS:HD2	1:C:70:ASN:H	1.03	1.01
2:C:481:HEM:HHH	2:C:481:HEM:HBC2	1.43	1.01
1:D:45:ILE:HG23	1:D:46:ILE:HD12	1.39	1.00
1:C:239:LEU:O	1:C:243:ILE:HG13	1.60	0.99
1:D:321:GLU:OE1	1:D:340:PHE:HB3	1.62	0.99
1:A:119:TYR:CD1	1:A:120:PRO:N	2.30	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:PRO:O	1:C:312:LYS:HG3	1.61	0.98
1:C:451:LEU:HD12	1:C:452:PRO:HD2	1.45	0.98
1:D:387:HIS:C	1:D:388:GLN:HE21	1.66	0.98
1:D:214:LEU:N	1:D:214:LEU:HD22	1.70	0.97
1:A:451:LEU:HD12	1:A:452:PRO:HD2	1.44	0.96
1:A:48:PHE:CD1	1:A:69:MET:HE3	1.99	0.95
1:D:446:GLU:O	1:D:470:VAL:HG13	1.66	0.95
1:B:188:ARG:HA	1:B:191:LEU:O	1.66	0.95
1:A:309:PRO:O	1:A:312:LYS:HG3	1.66	0.94
1:D:214:LEU:N	1:D:214:LEU:CD2	2.30	0.94
1:C:142:ALA:HB3	1:C:143:PRO:HD3	1.46	0.94
1:D:61:LYS:HE2	1:D:61:LYS:HA	1.49	0.94
1:D:388:GLN:HE21	1:D:388:GLN:HA	1.28	0.94
1:D:415:PHE:HE2	2:D:481:HEM:HBB2	1.33	0.94
1:B:72:CYS:SG	1:C:219:LYS:NZ	2.41	0.94
1:C:252:GLN:NE2	1:C:254:ASP:CB	2.30	0.93
1:C:252:GLN:HE21	1:C:254:ASP:HB3	1.27	0.93
1:A:120:PRO:HD2	1:A:121:ARG:H	1.34	0.93
3:B:490:TPF:F2	3:B:490:TPF:HC52	1.59	0.93
1:C:41:PHE:HB3	4:C:1:N8E:H232	1.50	0.92
1:D:312:LYS:HB2	1:D:313:ARG:NH2	1.84	0.92
1:D:334:VAL:HA	1:D:338:MET:CG	1.99	0.92
1:C:244:ILE:HD13	1:C:244:ILE:H	1.36	0.91
1:B:35:VAL:HG23	1:B:44:HIS:CE1	2.04	0.91
1:D:288:MET:HA	1:D:288:MET:CE	2.00	0.91
1:D:388:GLN:NE2	1:D:388:GLN:CA	2.31	0.91
1:D:367:GLN:HE21	1:D:367:GLN:H	1.15	0.90
1:D:388:GLN:NE2	1:D:388:GLN:HA	1.85	0.90
1:B:44:HIS:HD2	1:B:70:ASN:H	1.16	0.90
1:A:41:PHE:HD2	1:C:42:VAL:HG21	1.37	0.90
1:B:367:GLN:HE21	1:B:367:GLN:N	1.69	0.90
1:A:44:HIS:HD2	1:A:70:ASN:H	1.10	0.89
1:A:41:PHE:CD2	1:C:42:VAL:CG2	2.54	0.89
1:B:325:PHE:CE2	1:B:333:ASN:HB2	2.07	0.89
1:D:99:ARG:HH22	1:D:118:PRO:HA	1.37	0.89
1:D:214:LEU:O	1:D:217:ILE:HG23	1.72	0.89
1:D:213:PHE:C	1:D:214:LEU:CD2	2.40	0.88
1:A:138:PHE:CD1	1:A:430:LEU:HD22	2.07	0.88
1:B:455:ASN:C	1:B:455:ASN:HD22	1.76	0.88
1:A:142:ALA:HB3	1:A:143:PRO:HD3	1.53	0.88
1:A:118:PRO:C	1:A:120:PRO:HD2	1.95	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PHE:CD1	1:A:430:LEU:CD2	2.58	0.87
4:C:1:N8E:H012	4:C:1:N8E:H052	1.57	0.86
1:D:334:VAL:HA	1:D:338:MET:HG3	1.57	0.86
1:C:42:VAL:HG11	1:C:46:ILE:HD13	1.58	0.86
1:D:292:GLN:O	1:D:296:THR:HG22	1.75	0.86
1:D:387:HIS:C	1:D:388:GLN:NE2	2.30	0.85
1:C:128:PHE:HD1	1:C:275:MET:CE	1.89	0.85
1:A:119:TYR:N	1:A:120:PRO:CD	2.40	0.85
1:A:101:VAL:HG12	1:A:102:TYR:CD1	2.11	0.85
1:B:335:MET:HA	1:B:335:MET:CE	2.07	0.84
1:C:240:SER:O	1:C:244:ILE:CD1	2.25	0.84
1:C:252:GLN:CD	1:C:254:ASP:H	1.80	0.84
1:B:292:GLN:O	1:B:296:THR:CG2	2.25	0.84
1:C:453:GLU:HG3	1:C:454:PRO:HD2	1.58	0.84
1:C:135:VAL:HA	1:C:138:PHE:CD2	2.13	0.83
1:C:44:HIS:CD2	1:C:70:ASN:H	1.92	0.83
1:C:42:VAL:HG13	1:C:45:ILE:HG22	1.61	0.83
1:A:120:PRO:CD	1:A:121:ARG:H	1.92	0.82
1:C:32:PRO:HA	1:C:371:TYR:CD2	2.15	0.82
1:C:476:LYS:HB3	1:C:476:LYS:NZ	1.95	0.81
1:B:455:ASN:ND2	1:B:457:HIS:H	1.77	0.81
1:A:42:VAL:HG21	1:C:40:PRO:CB	2.09	0.81
1:A:42:VAL:CG2	1:C:40:PRO:HB2	2.09	0.81
1:A:48:PHE:HD1	1:A:69:MET:HE3	1.42	0.81
1:B:330:ASN:HD22	1:B:331:TYR:H	1.28	0.81
3:C:490:TPF:F2	3:C:490:TPF:HC52	1.70	0.81
1:D:138:PHE:HD2	1:D:430:LEU:HD22	1.45	0.81
1:D:388:GLN:NE2	1:D:388:GLN:N	2.29	0.81
1:B:101:VAL:HG12	1:B:102:TYR:CD1	2.16	0.81
1:A:48:PHE:CD1	1:A:69:MET:CE	2.64	0.80
1:B:44:HIS:CD2	1:B:70:ASN:H	1.98	0.80
1:C:128:PHE:HD1	1:C:275:MET:HE3	1.46	0.80
1:A:119:TYR:N	1:A:120:PRO:HD3	1.94	0.80
1:A:452:PRO:HA	1:A:467:GLN:OE1	1.81	0.80
1:C:200:LEU:O	1:C:204:GLU:HG3	1.80	0.80
1:C:240:SER:O	1:C:244:ILE:HD11	1.80	0.80
1:C:42:VAL:HG13	1:C:45:ILE:CG2	2.12	0.80
4:C:1:N8E:H172	1:D:220:LEU:HD22	1.63	0.80
1:A:41:PHE:HD2	1:C:42:VAL:CG2	1.92	0.80
1:C:89:PHE:CG	1:C:417:ALA:HB3	2.16	0.79
1:A:139:GLN:OE1	1:A:140:ASN:N	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:THR:HB	1:A:40:PRO:HD2	1.66	0.78
1:D:135:VAL:HA	1:D:138:PHE:CD1	2.17	0.78
1:C:254:ASP:O	1:C:255:THR:HB	1.82	0.78
1:D:214:LEU:O	1:D:217:ILE:CG2	2.31	0.78
3:D:490:TPF:HC52	3:D:490:TPF:F2	1.71	0.78
1:B:101:VAL:HG12	1:B:102:TYR:HD1	1.47	0.78
1:D:293:HIS:HA	1:D:296:THR:CG2	2.14	0.78
1:A:191:LEU:HD21	1:A:196:PHE:HD2	1.46	0.78
1:B:182:LEU:O	1:B:259:ASP:HB2	1.84	0.78
1:B:250:GLU:O	1:B:253:LYS:CG	2.32	0.78
1:A:41:PHE:CD2	1:C:42:VAL:HG21	2.16	0.77
1:A:42:VAL:CG1	1:A:45:ILE:HG23	2.15	0.77
1:B:350:ARG:O	1:B:350:ARG:HD2	1.84	0.77
1:A:119:TYR:CD1	1:A:119:TYR:C	2.58	0.77
1:D:61:LYS:CA	1:D:61:LYS:HE2	2.15	0.77
1:B:330:ASN:H	1:B:333:ASN:HD21	0.80	0.77
1:C:254:ASP:O	1:C:255:THR:CB	2.33	0.77
1:A:203:MET:O	1:A:228:CYS:SG	2.43	0.77
2:D:481:HEM:HBC2	2:D:481:HEM:HMC1	1.67	0.76
1:B:330:ASN:HB3	1:B:333:ASN:OD1	1.85	0.76
1:C:42:VAL:CG1	1:C:45:ILE:HG22	2.15	0.76
1:A:182:LEU:O	1:A:259:ASP:HB2	1.86	0.76
1:D:334:VAL:HG13	1:D:338:MET:SD	2.26	0.76
1:C:204:GLU:OE1	1:C:293:HIS:CE1	2.39	0.76
1:C:182:LEU:HD12	1:C:288:MET:HE1	1.68	0.76
1:D:28:LYS:HD3	1:D:28:LYS:C	2.05	0.76
1:A:42:VAL:HG11	1:A:46:ILE:HD13	1.68	0.76
1:B:95:ILE:N	1:B:95:ILE:HD12	2.01	0.75
1:D:350:ARG:HD2	1:D:350:ARG:O	1.85	0.75
1:D:367:GLN:NE2	1:D:367:GLN:N	2.31	0.75
1:B:367:GLN:HE21	1:B:367:GLN:H	1.34	0.75
1:D:148:GLU:HB2	1:D:177:THR:HG22	1.65	0.75
1:D:69:MET:HB2	1:D:76:ILE:HG23	1.67	0.75
1:A:155:ALA:C	1:A:156:ASN:HD22	1.89	0.75
1:C:179:CYS:O	1:C:183:PHE:HB2	1.86	0.75
1:A:199:LEU:HD13	1:A:235:LEU:HB2	1.67	0.75
3:A:490:TPF:O	3:A:490:TPF:HC6	1.86	0.74
3:C:490:TPF:HC6	3:C:490:TPF:O	1.87	0.74
1:C:292:GLN:O	1:C:296:THR:CG2	2.33	0.74
1:D:142:ALA:HB3	1:D:143:PRO:HD3	1.69	0.74
1:A:118:PRO:C	1:A:120:PRO:CD	2.55	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PHE:CE1	1:A:430:LEU:CD2	2.71	0.74
1:B:455:ASN:HD21	1:B:457:HIS:HB2	1.53	0.74
1:D:208:ILE:HG21	1:D:217:ILE:HD11	1.70	0.73
1:C:95:ILE:HD12	1:C:95:ILE:N	2.02	0.73
4:C:1:N8E:H013	1:D:45:ILE:CD1	2.18	0.73
1:A:42:VAL:HG21	1:C:40:PRO:HB2	1.68	0.73
1:A:119:TYR:HD1	1:A:120:PRO:N	1.87	0.73
1:A:471:LYS:HE2	1:A:473:ILE:HD11	1.70	0.73
1:C:308:ASP:OD2	1:C:310:ARG:NH2	2.21	0.72
3:A:490:TPF:HC52	3:A:490:TPF:F2	1.79	0.72
1:B:192:ASP:OD2	1:B:195:GLN:HG3	1.89	0.72
2:D:481:HEM:HBC2	2:D:481:HEM:CMC	2.19	0.72
1:C:135:VAL:HA	1:C:138:PHE:CE2	2.24	0.72
1:C:128:PHE:O	1:C:132:GLU:HG2	1.89	0.72
1:C:48:PHE:CD1	1:C:69:MET:CE	2.72	0.71
1:D:213:PHE:O	1:D:214:LEU:HD22	1.88	0.71
1:A:118:PRO:O	1:A:120:PRO:HD2	1.89	0.71
1:A:453:GLU:HG3	1:A:454:PRO:HD2	1.72	0.71
1:A:475:LYS:O	1:A:476:LYS:CB	2.39	0.71
1:C:475:LYS:O	1:C:476:LYS:O	2.09	0.71
1:A:350:ARG:O	1:A:350:ARG:HD2	1.91	0.71
1:A:42:VAL:HG13	1:A:45:ILE:HG23	1.71	0.71
1:C:48:PHE:CD1	1:C:69:MET:HE3	2.25	0.71
1:D:67:PHE:CZ	1:D:78:VAL:HG21	2.25	0.70
1:A:206:CYS:HA	1:A:224:GLN:HB3	1.72	0.70
1:C:387:HIS:HE1	1:C:413:CYS:H	1.39	0.70
1:D:350:ARG:HA	1:D:387:HIS:CD2	2.26	0.70
1:A:72:CYS:SG	1:A:214:LEU:HD11	2.31	0.70
1:B:250:GLU:O	1:B:253:LYS:HG3	1.90	0.70
1:B:424:GLY:HA3	2:B:481:HEM:C3C	2.26	0.70
1:A:234:GLU:OE2	1:B:469:ARG:NH1	2.24	0.70
1:A:128:PHE:HD1	1:A:275:MET:CE	2.04	0.70
1:A:206:CYS:CB	1:A:228:CYS:SG	2.77	0.70
1:B:35:VAL:CG2	1:B:44:HIS:CE1	2.74	0.70
1:C:455:ASN:ND2	1:C:457:HIS:HD2	1.90	0.70
1:A:139:GLN:C	1:A:139:GLN:OE1	2.30	0.70
1:C:455:ASN:HD21	1:C:457:HIS:HD2	1.38	0.70
1:C:246:ARG:O	1:C:250:GLU:HB2	1.92	0.70
1:C:99:ARG:HD2	1:C:115:TYR:O	1.90	0.70
1:A:451:LEU:HD12	1:A:452:PRO:CD	2.21	0.70
1:B:214:LEU:O	1:B:217:ILE:HG22	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:ALA:HB2	1:D:408:VAL:HG21	1.73	0.69
1:A:292:GLN:O	1:A:296:THR:CG2	2.35	0.69
1:C:455:ASN:HD21	1:C:457:HIS:CD2	2.10	0.69
1:A:206:CYS:O	1:A:208:ILE:HG13	1.92	0.69
1:C:81:ASP:OD1	1:C:81:ASP:C	2.30	0.69
1:B:335:MET:HE3	1:B:335:MET:HA	1.73	0.69
3:A:490:TPF:C6	3:A:490:TPF:O	2.40	0.68
1:B:330:ASN:ND2	1:B:331:TYR:H	1.90	0.68
1:B:258:SER:HB3	1:B:262:ALA:HB3	1.74	0.68
1:A:235:LEU:CD2	1:A:285:VAL:HG22	2.23	0.68
1:A:476:LYS:HD3	1:A:476:LYS:C	2.13	0.68
1:B:317:LYS:NZ	1:B:402:GLU:OE2	2.22	0.68
1:B:455:ASN:C	1:B:455:ASN:ND2	2.46	0.68
1:C:190:ARG:NH2	1:C:241:GLU:OE1	2.26	0.68
1:A:82:VAL:HG22	1:A:411:ALA:HA	1.75	0.68
1:A:138:PHE:CE1	1:A:430:LEU:HD22	2.29	0.68
1:B:142:ALA:HB3	1:B:143:PRO:HD3	1.74	0.68
3:C:490:TPF:O	3:C:490:TPF:C6	2.39	0.68
1:D:138:PHE:CD2	1:D:430:LEU:HD22	2.27	0.68
1:A:190:ARG:HA	1:B:163:GLU:OE2	1.93	0.68
1:D:154:LYS:HG2	1:D:154:LYS:O	1.94	0.68
1:A:370:LYS:HE3	1:A:371:TYR:CZ	2.29	0.68
1:D:407:LEU:C	1:D:407:LEU:CD1	2.55	0.68
1:A:101:VAL:HG12	1:A:102:TYR:HD1	1.58	0.67
1:A:42:VAL:HG13	1:A:45:ILE:CG2	2.24	0.67
1:D:444:ASP:HB2	1:D:473:ILE:HB	1.75	0.67
1:D:415:PHE:CE2	2:D:481:HEM:HBB2	2.23	0.67
1:C:350:ARG:O	1:C:350:ARG:HD2	1.93	0.67
1:D:39:THR:HB	1:D:40:PRO:HD2	1.77	0.67
1:A:44:HIS:CD2	1:A:70:ASN:H	2.03	0.67
1:C:101:VAL:HG11	1:C:359:MET:HB2	1.75	0.67
1:B:455:ASN:HD22	1:B:457:HIS:H	1.43	0.66
1:A:40:PRO:HG3	1:C:39:THR:HB	1.78	0.66
1:D:407:LEU:O	1:D:407:LEU:CD1	2.30	0.66
1:A:76:ILE:HD11	1:A:357:MET:HE1	1.78	0.66
1:A:424:GLY:HA3	2:A:481:HEM:C3C	2.30	0.66
1:B:84:GLN:OE1	1:B:87:LYS:HE2	1.96	0.66
1:C:253:LYS:HG3	1:C:253:LYS:O	1.94	0.66
1:A:39:THR:CB	1:A:40:PRO:HD2	2.25	0.66
1:B:314:HIS:CE1	1:B:401:PRO:HD2	2.30	0.66
1:B:216:TRP:CZ3	1:C:216:TRP:HB3	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ILE:HD11	1:B:469:ARG:CD	2.26	0.66
1:C:206:CYS:HB2	1:C:228:CYS:HB2	1.78	0.66
1:B:288:MET:HA	1:B:288:MET:HE2	1.78	0.66
1:B:250:GLU:O	1:B:253:LYS:HG2	1.95	0.66
1:C:41:PHE:CB	4:C:1:N8E:H232	2.23	0.66
1:A:138:PHE:CE1	1:A:430:LEU:HD23	2.31	0.65
1:B:119:TYR:HB2	1:B:120:PRO:HD3	1.75	0.65
1:C:400:ASN:O	1:C:403:ARG:HG2	1.96	0.65
1:D:154:LYS:C	5:D:482:HOH:O	2.34	0.65
1:C:252:GLN:OE1	1:C:253:LYS:N	2.30	0.65
1:C:42:VAL:CG1	1:C:46:ILE:HD13	2.25	0.65
1:D:28:LYS:HD3	1:D:29:GLY:N	2.12	0.65
1:B:254:ASP:OD1	1:B:254:ASP:N	2.30	0.65
1:B:453:GLU:HG3	1:B:454:PRO:HD2	1.79	0.65
1:C:155:ALA:C	1:C:156:ASN:HD22	2.01	0.64
1:A:213:PHE:C	1:A:214:LEU:HD12	2.18	0.64
1:A:42:VAL:HG21	1:C:40:PRO:HB3	1.77	0.64
1:C:121:ARG:O	1:C:125:GLN:HG3	1.98	0.64
1:D:387:HIS:O	1:D:388:GLN:NE2	2.30	0.64
1:A:39:THR:OG1	1:A:42:VAL:HB	1.98	0.64
1:D:51:ASP:OD2	1:D:54:GLY:HA3	1.96	0.64
1:C:331:TYR:CE1	1:C:335:MET:HG3	2.32	0.64
1:B:135:VAL:HA	1:B:138:PHE:CD2	2.32	0.64
1:D:442:ASP:O	1:D:475:LYS:HG2	1.98	0.64
1:C:223:PRO:HA	1:C:226:TYR:HD2	1.61	0.64
1:A:50:LYS:HD3	1:A:50:LYS:C	2.18	0.64
1:D:334:VAL:CA	1:D:338:MET:HG3	2.28	0.64
1:B:304:LEU:HD13	1:B:452:PRO:HG2	1.79	0.63
1:C:309:PRO:O	1:C:312:LYS:CG	2.40	0.63
1:A:415:PHE:CE2	1:A:425:GLU:HG3	2.34	0.63
1:D:472:TYR:O	1:D:472:TYR:CD1	2.52	0.63
1:C:475:LYS:O	1:C:476:LYS:C	2.35	0.63
1:C:206:CYS:CB	1:C:228:CYS:HB2	2.29	0.63
1:B:135:VAL:HB	1:B:331:TYR:OH	1.98	0.63
1:D:473:ILE:HD12	1:D:473:ILE:N	2.13	0.63
1:C:81:ASP:OD1	1:C:83:HIS:N	2.30	0.63
1:A:42:VAL:HG23	1:C:40:PRO:HB2	1.79	0.63
3:B:490:TPF:HC6	3:B:490:TPF:O	1.99	0.63
4:C:1:N8E:H013	1:D:45:ILE:HD11	1.81	0.63
1:C:476:LYS:HZ2	1:C:476:LYS:HB3	1.63	0.63
1:C:95:ILE:HG21	1:C:366:VAL:CG1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:LEU:HD22	2:D:481:HEM:CGA	2.28	0.63
1:A:135:VAL:HA	1:A:138:PHE:CD2	2.33	0.62
1:C:128:PHE:HD1	1:C:275:MET:HE2	1.63	0.62
1:C:141:PHE:O	1:C:145:ILE:HG13	1.98	0.62
1:C:145:ILE:O	1:C:149:VAL:HG23	1.98	0.62
1:D:395:ASN:N	1:D:396:PRO:HD3	2.14	0.62
1:B:105:MET:CE	1:B:109:PHE:CZ	2.83	0.62
1:B:330:ASN:HD22	1:B:331:TYR:N	1.95	0.62
1:D:223:PRO:HA	1:D:226:TYR:HD2	1.65	0.62
1:A:288:MET:HE2	1:A:288:MET:HA	1.81	0.62
1:A:384:LEU:O	1:A:388:GLN:HG2	1.99	0.62
1:D:106:VAL:N	1:D:107:PRO:CD	2.62	0.62
1:A:89:PHE:CG	1:A:417:ALA:HB3	2.35	0.62
1:B:105:MET:HE2	1:B:109:PHE:CZ	2.34	0.62
1:A:94:GLU:O	1:A:363:LEU:HD12	2.00	0.62
1:B:42:VAL:HB	1:B:45:ILE:CG2	2.29	0.62
1:A:82:VAL:CG2	1:A:411:ALA:HA	2.30	0.62
1:A:177:THR:OG1	1:A:431:GLN:NE2	2.33	0.62
1:B:331:TYR:CE1	1:B:335:MET:HG3	2.35	0.62
1:D:304:LEU:HD13	1:D:452:PRO:HG2	1.82	0.62
1:D:128:PHE:CD2	1:D:267:ALA:HB1	2.35	0.61
1:A:406:LYS:HD2	1:A:409:ASP:OD2	2.00	0.61
2:C:481:HEM:HBC2	2:C:481:HEM:CHD	2.21	0.61
1:D:41:PHE:CD1	1:D:41:PHE:O	2.54	0.61
1:D:39:THR:OG1	1:D:42:VAL:HG12	2.01	0.61
1:C:331:TYR:CZ	1:C:335:MET:HG3	2.35	0.61
1:C:51:ASP:OD1	1:C:54:GLY:HA3	2.00	0.61
1:B:350:ARG:C	1:B:350:ARG:HD2	2.20	0.61
1:C:31:LEU:HD22	1:C:374:PRO:HD3	1.83	0.61
1:B:177:THR:OG1	1:B:431:GLN:NE2	2.33	0.61
1:C:128:PHE:CD1	1:C:275:MET:HE3	2.31	0.61
1:C:111:GLU:O	1:C:278:HIS:HE1	1.84	0.61
1:C:93:ASN:HA	1:C:96:LEU:O	2.00	0.61
1:A:238:ILE:HD11	1:B:469:ARG:NE	2.15	0.60
1:D:204:GLU:OE1	1:D:293:HIS:NE2	2.32	0.60
3:D:490:TPF:O	3:D:490:TPF:HC6	2.00	0.60
1:A:209:PRO:O	1:A:212:VAL:CG2	2.30	0.60
1:A:355:LEU:HD11	3:A:490:TPF:N4	2.15	0.60
1:D:339:PRO:O	1:D:343:GLN:HG3	2.01	0.60
1:C:207:LEU:HD13	1:C:459:MET:SD	2.41	0.60
1:B:45:ILE:HG23	1:B:46:ILE:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:PHE:CD1	1:C:275:MET:CE	2.80	0.60
1:C:252:GLN:CD	1:C:254:ASP:N	2.54	0.60
1:C:31:LEU:CD2	1:C:374:PRO:HD3	2.32	0.60
1:A:35:VAL:O	1:A:44:HIS:CE1	2.55	0.59
1:C:297:ILE:CD1	1:C:460:VAL:HG12	2.32	0.59
1:D:453:GLU:HG3	1:D:454:PRO:HD2	1.83	0.59
1:A:287:ALA:HB1	2:A:481:HEM:HBC1	1.84	0.59
1:C:306:LEU:HD13	1:C:440:LEU:HD11	1.84	0.59
1:A:42:VAL:CG1	1:A:45:ILE:CG2	2.81	0.59
1:B:290:ALA:HB1	3:B:490:TPF:C7	2.33	0.59
1:C:452:PRO:HA	1:C:467:GLN:OE1	2.02	0.59
1:D:288:MET:CE	1:D:288:MET:CA	2.79	0.59
1:D:101:VAL:HG11	1:D:359:MET:HB2	1.85	0.59
1:A:39:THR:HB	1:A:40:PRO:CD	2.32	0.59
1:B:170:CYS:O	1:B:174:ILE:HG12	2.03	0.59
1:B:470:VAL:CG1	1:B:471:LYS:N	2.66	0.59
1:C:422:CYS:HB2	2:C:481:HEM:NA	2.17	0.59
1:D:141:PHE:O	1:D:145:ILE:HG13	2.02	0.58
1:D:53:LEU:O	1:D:57:LEU:HB2	2.03	0.58
1:A:120:PRO:CD	1:A:121:ARG:N	2.59	0.58
1:A:145:ILE:O	1:A:149:VAL:HG23	2.04	0.58
1:A:128:PHE:HD1	1:A:275:MET:HE3	1.66	0.58
1:D:321:GLU:OE1	1:D:340:PHE:CB	2.47	0.58
1:C:142:ALA:HB3	1:C:143:PRO:CD	2.27	0.58
1:D:334:VAL:CA	1:D:338:MET:SD	2.81	0.58
1:B:333:ASN:O	1:B:338:MET:HG3	2.04	0.58
1:B:350:ARG:HA	1:B:387:HIS:CD2	2.39	0.58
1:C:291:GLY:O	1:C:295:SER:HB2	2.04	0.58
1:D:313:ARG:H	1:D:313:ARG:NE	2.02	0.58
1:A:40:PRO:HG3	1:C:39:THR:CB	2.34	0.58
1:C:82:VAL:O	1:C:82:VAL:HG13	2.02	0.58
1:A:475:LYS:O	1:A:476:LYS:HB3	2.04	0.58
3:B:490:TPF:C6	3:B:490:TPF:O	2.51	0.58
1:D:392:ALA:HB2	1:D:408:VAL:CG2	2.33	0.58
1:C:51:ASP:OD2	1:C:52:PRO:HD2	2.03	0.57
1:D:149:VAL:O	1:D:153:MET:HG3	2.04	0.57
1:D:300:THR:O	1:D:304:LEU:HG	2.03	0.57
1:A:98:PRO:HG3	1:A:420:HIS:CE1	2.39	0.57
1:B:335:MET:HA	1:B:335:MET:HE2	1.86	0.57
1:B:95:ILE:N	1:B:95:ILE:CD1	2.65	0.57
1:C:112:GLY:HA2	1:C:116:ALA:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:ASP:O	1:C:255:THR:HG22	2.03	0.57
1:B:214:LEU:O	1:B:217:ILE:CG2	2.52	0.57
1:D:214:LEU:HB3	1:D:217:ILE:HG22	1.85	0.57
1:A:111:GLU:CD	1:D:40:PRO:O	2.43	0.57
1:C:387:HIS:CE1	1:C:413:CYS:H	2.21	0.57
1:D:137:LYS:C	1:D:139:GLN:OE1	2.43	0.57
1:D:330:ASN:OD1	1:D:330:ASN:C	2.43	0.57
1:A:86:SER:O	1:A:90:THR:HB	2.02	0.57
1:B:76:ILE:HA	1:B:378:ILE:O	2.04	0.57
1:C:325:PHE:HB3	1:C:329:LEU:HD21	1.86	0.57
1:C:422:CYS:HB2	2:C:481:HEM:C4A	2.40	0.57
1:B:347:GLU:OE1	1:B:403:ARG:HD2	2.05	0.57
3:D:490:TPF:C6	3:D:490:TPF:O	2.53	0.57
1:D:93:ASN:HA	1:D:96:LEU:O	2.05	0.57
1:C:240:SER:O	1:C:244:ILE:HD13	2.02	0.57
1:A:338:MET:HE1	1:A:437:ALA:HB2	1.85	0.57
1:C:370:LYS:HE2	1:C:371:TYR:CZ	2.40	0.57
1:B:182:LEU:CD1	1:B:288:MET:HE3	2.35	0.57
1:C:32:PRO:HA	1:C:371:TYR:CE2	2.40	0.57
1:A:173:MET:O	1:A:177:THR:HG23	2.05	0.57
1:A:350:ARG:HA	1:A:387:HIS:CD2	2.40	0.56
1:C:244:ILE:HD13	1:C:244:ILE:N	2.15	0.56
1:C:254:ASP:C	1:C:255:THR:HG22	2.25	0.56
1:C:95:ILE:HD12	1:C:95:ILE:H	1.70	0.56
1:B:330:ASN:ND2	1:B:331:TYR:N	2.52	0.56
1:C:33:PRO:HD3	1:C:371:TYR:CE2	2.40	0.56
1:C:314:HIS:CE1	1:C:401:PRO:HD2	2.40	0.56
1:A:45:ILE:HG12	1:A:46:ILE:N	2.17	0.56
1:C:288:MET:CE	1:C:288:MET:HA	2.35	0.56
1:D:36:HIS:CD2	1:D:37:GLY:H	2.23	0.56
1:D:347:GLU:HA	1:D:405:MET:HE1	1.85	0.56
1:B:71:ILE:HG21	1:B:213:PHE:CD1	2.41	0.56
1:D:239:LEU:O	1:D:243:ILE:HG13	2.05	0.56
1:D:45:ILE:CG2	1:D:46:ILE:HD12	2.26	0.56
1:B:182:LEU:HD13	1:B:288:MET:HE3	1.86	0.56
1:C:252:GLN:OE1	1:C:254:ASP:N	2.30	0.56
1:C:254:ASP:O	1:C:255:THR:CG2	2.53	0.56
1:C:82:VAL:HG11	1:C:408:VAL:HG11	1.88	0.56
1:C:446:GLU:O	1:C:470:VAL:HG13	2.04	0.56
1:D:104:PHE:HA	1:D:218:LEU:HD11	1.86	0.56
1:A:42:VAL:CG1	1:A:46:ILE:HD13	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:GLU:CD	1:D:100:GLU:H	2.09	0.56
1:A:76:ILE:HG23	1:A:76:ILE:O	2.06	0.56
1:C:45:ILE:HG23	1:C:46:ILE:N	2.20	0.56
1:A:281:CYS:O	1:A:285:VAL:HG23	2.04	0.56
1:D:35:VAL:HG12	1:D:68:THR:O	2.06	0.56
1:A:120:PRO:O	1:A:124:GLU:HG3	2.06	0.56
1:A:139:GLN:C	1:A:139:GLN:CD	2.65	0.56
1:B:106:VAL:N	1:B:107:PRO:CD	2.69	0.56
1:B:42:VAL:HB	1:B:45:ILE:HG22	1.88	0.56
1:D:350:ARG:HD2	1:D:350:ARG:C	2.25	0.56
1:A:206:CYS:O	1:A:207:LEU:C	2.44	0.56
1:A:350:ARG:O	1:A:387:HIS:HB3	2.06	0.56
1:C:195:GLN:NE2	1:D:163:GLU:O	2.37	0.56
1:A:101:VAL:CG1	1:A:102:TYR:CD1	2.87	0.55
1:C:101:VAL:HG13	1:C:359:MET:HE3	1.86	0.55
1:D:387:HIS:HE1	1:D:413:CYS:H	1.52	0.55
1:D:61:LYS:CA	1:D:61:LYS:CE	2.82	0.55
1:B:252:GLN:HA	1:B:252:GLN:OE1	2.07	0.55
1:B:356:VAL:HG21	1:B:461:VAL:HG21	1.87	0.55
1:C:395:ASN:N	1:C:396:PRO:HD3	2.21	0.55
1:C:82:VAL:HG12	1:C:83:HIS:N	2.21	0.55
1:D:134:THR:C	1:D:138:PHE:HE1	2.09	0.55
1:D:169:ASP:O	1:D:173:MET:HG3	2.06	0.55
1:D:281:CYS:O	1:D:285:VAL:HG23	2.06	0.55
1:D:293:HIS:O	1:D:296:THR:HG23	2.06	0.55
1:B:240:SER:O	1:B:244:ILE:HG12	2.07	0.55
1:C:384:LEU:O	1:C:388:GLN:HG2	2.06	0.55
1:D:44:HIS:HD2	1:D:70:ASN:H	1.54	0.55
1:A:120:PRO:HD2	1:A:121:ARG:N	2.13	0.55
1:B:213:PHE:O	1:B:214:LEU:HD12	2.07	0.55
1:B:325:PHE:CE2	1:B:333:ASN:CB	2.85	0.55
2:C:481:HEM:HAD1	3:C:490:TPF:H10	1.88	0.55
1:C:67:PHE:CZ	1:C:78:VAL:HG21	2.42	0.55
1:D:190:ARG:O	1:D:190:ARG:HD2	2.05	0.55
1:A:472:TYR:C	1:A:473:ILE:HD12	2.27	0.55
1:C:175:ILE:HG12	1:C:197:ALA:HB2	1.88	0.55
1:C:206:CYS:SG	1:C:225:SER:HA	2.47	0.55
1:C:243:ILE:O	1:C:246:ARG:HB2	2.06	0.55
1:C:415:PHE:CE2	1:C:425:GLU:HG3	2.42	0.55
1:B:67:PHE:CZ	1:B:78:VAL:HG21	2.41	0.55
1:C:476:LYS:HZ3	1:C:476:LYS:HB3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:GLU:OE1	1:D:289:PHE:CD1	2.59	0.55
1:A:358:LEU:HD22	2:A:481:HEM:HBA2	1.89	0.55
1:B:355:LEU:HD11	3:B:490:TPF:N4	2.21	0.55
1:D:138:PHE:HE2	1:D:427:PHE:HA	1.72	0.55
1:C:252:GLN:NE2	1:C:254:ASP:CA	2.69	0.55
1:C:355:LEU:HD11	3:C:490:TPF:N4	2.21	0.54
1:C:48:PHE:CD1	1:C:69:MET:HE1	2.41	0.54
1:D:443:TYR:OH	1:D:474:LYS:NZ	2.40	0.54
1:B:138:PHE:CD1	1:B:141:PHE:CD2	2.95	0.54
1:C:106:VAL:N	1:C:107:PRO:CD	2.69	0.54
1:C:206:CYS:O	1:C:208:ILE:HG13	2.07	0.54
1:C:475:LYS:HA	1:C:475:LYS:HE3	1.89	0.54
1:D:455:ASN:ND2	1:D:457:HIS:H	2.04	0.54
1:D:135:VAL:CA	1:D:138:PHE:CD1	2.89	0.54
1:D:45:ILE:HG23	1:D:46:ILE:CD1	2.25	0.54
4:C:1:N8E:C01	4:C:1:N8E:H052	2.35	0.54
1:C:51:ASP:CG	1:C:54:GLY:H	2.10	0.54
1:D:146:GLN:HE22	1:D:329:LEU:HG	1.73	0.54
1:C:196:PHE:CZ	1:C:288:MET:HG3	2.43	0.54
1:D:303:LEU:O	1:D:307:MET:HG2	2.07	0.54
1:D:82:VAL:HG21	1:D:411:ALA:HB1	1.89	0.54
1:D:42:VAL:HG22	1:D:45:ILE:CG2	2.38	0.54
1:C:95:ILE:CG2	1:C:366:VAL:CG1	2.85	0.54
1:D:331:TYR:CE1	1:D:335:MET:HG3	2.42	0.54
1:A:41:PHE:CD2	1:C:42:VAL:HG22	2.42	0.54
1:C:420:HIS:HA	2:C:481:HEM:O2D	2.08	0.54
1:D:160:ASP:N	1:D:160:ASP:OD2	2.40	0.54
1:A:139:GLN:OE1	1:A:140:ASN:CB	2.56	0.54
1:D:38:THR:HB	1:D:44:HIS:NE2	2.23	0.54
1:A:465:ALA:O	1:A:468:CYS:HB2	2.07	0.54
1:C:109:PHE:O	1:C:232:ARG:NH2	2.40	0.54
1:B:470:VAL:HG12	1:B:471:LYS:N	2.22	0.53
1:D:213:PHE:HB2	1:D:214:LEU:CD2	2.38	0.53
1:A:149:VAL:O	1:A:153:MET:HG3	2.08	0.53
1:A:331:TYR:CE1	1:A:335:MET:HG3	2.43	0.53
1:C:35:VAL:HG12	1:C:68:THR:O	2.08	0.53
1:D:135:VAL:HA	1:D:138:PHE:CE1	2.43	0.53
1:B:209:PRO:O	1:B:212:VAL:HG23	2.09	0.53
1:B:387:HIS:HE1	1:B:413:CYS:H	1.55	0.53
1:B:395:ASN:OD1	1:B:398:GLU:OE1	2.26	0.53
1:D:240:SER:O	1:D:244:ILE:HG13	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:HIS:HA	1:D:296:THR:HG22	1.88	0.53
1:C:223:PRO:HA	1:C:226:TYR:CD2	2.43	0.53
1:A:302:SER:O	1:A:306:LEU:HG	2.07	0.53
1:A:322:ILE:HA	1:A:325:PHE:HD1	1.72	0.53
1:A:39:THR:CB	1:A:40:PRO:CD	2.86	0.53
1:A:288:MET:CA	1:A:288:MET:HE2	2.38	0.53
1:B:319:HIS:O	1:B:323:ASP:CG	2.46	0.53
1:B:330:ASN:O	1:B:333:ASN:ND2	2.41	0.53
1:D:472:TYR:C	1:D:472:TYR:CD1	2.82	0.53
1:A:101:VAL:O	1:A:101:VAL:HG13	2.09	0.53
1:C:69:MET:HB2	1:C:76:ILE:HG23	1.89	0.53
1:D:243:ILE:O	1:D:247:GLU:HG3	2.09	0.53
1:A:387:HIS:HE1	1:A:413:CYS:H	1.56	0.53
1:C:325:PHE:HB3	1:C:329:LEU:CD2	2.39	0.53
1:D:312:LYS:H	1:D:313:ARG:HH21	1.57	0.53
1:B:87:LYS:HD3	1:B:368:VAL:HA	1.91	0.53
1:A:138:PHE:CE1	1:A:427:PHE:HD1	2.27	0.52
1:A:55:PHE:CE2	1:A:69:MET:HE3	2.44	0.52
1:C:350:ARG:C	1:C:350:ARG:HD2	2.29	0.52
1:D:173:MET:O	1:D:177:THR:HG23	2.09	0.52
1:A:239:LEU:O	1:A:243:ILE:HG13	2.09	0.52
1:B:216:TRP:CG	1:C:215:PRO:HG2	2.45	0.52
1:C:244:ILE:CD1	1:C:244:ILE:H	2.04	0.52
1:C:383:PRO:O	1:C:387:HIS:CG	2.62	0.52
1:A:321:GLU:OE2	1:A:338:MET:HA	2.08	0.52
1:C:50:LYS:HD3	1:C:50:LYS:C	2.30	0.52
1:D:128:PHE:CE2	1:D:267:ALA:HB1	2.44	0.52
1:A:31:LEU:HD22	1:A:374:PRO:HD3	1.91	0.52
1:B:331:TYR:O	1:B:335:MET:HG2	2.10	0.52
1:B:400:ASN:O	1:B:403:ARG:HG2	2.10	0.52
1:B:65:GLY:O	1:B:80:GLY:N	2.42	0.52
1:C:119:TYR:N	1:C:120:PRO:HD2	2.24	0.52
1:C:301:TRP:NE1	1:C:463:PRO:HD3	2.24	0.52
1:C:48:PHE:HD1	1:C:69:MET:HE3	1.72	0.52
1:D:350:ARG:O	1:D:387:HIS:CD2	2.62	0.52
1:A:322:ILE:HA	1:A:325:PHE:CD1	2.45	0.52
1:C:101:VAL:O	1:C:101:VAL:HG12	2.10	0.52
1:A:156:ASN:HD22	1:A:156:ASN:N	2.03	0.52
1:A:200:LEU:O	1:A:204:GLU:HG2	2.10	0.52
1:A:224:GLN:HE22	1:B:224:GLN:HG2	1.74	0.52
1:A:309:PRO:O	1:A:312:LYS:CG	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ALA:O	1:B:175:ILE:HG22	2.09	0.52
2:D:481:HEM:HMC1	2:D:481:HEM:CBC	2.37	0.52
1:D:43:GLY:HA3	1:D:70:ASN:O	2.10	0.52
1:B:213:PHE:C	1:B:214:LEU:HD12	2.31	0.52
1:C:297:ILE:HD12	1:C:460:VAL:HG12	1.92	0.52
1:D:308:ASP:OD1	1:D:309:PRO:HD2	2.09	0.52
1:B:53:LEU:HD13	1:B:384:LEU:HG	1.91	0.51
1:B:82:VAL:HG22	1:B:411:ALA:HA	1.90	0.51
1:D:125:GLN:HA	1:D:128:PHE:CD1	2.46	0.51
1:A:415:PHE:CD2	1:A:425:GLU:HG3	2.45	0.51
1:C:39:THR:OG1	1:C:42:VAL:HB	2.10	0.51
1:A:224:GLN:NE2	1:B:224:GLN:HG2	2.24	0.51
1:D:298:THR:HG21	1:D:349:ILE:HD11	1.92	0.51
1:D:38:THR:HB	1:D:44:HIS:CE1	2.46	0.51
1:B:135:VAL:HA	1:B:138:PHE:CE2	2.46	0.51
1:B:424:GLY:HA3	2:B:481:HEM:C2C	2.45	0.51
1:D:322:ILE:HA	1:D:325:PHE:HD1	1.75	0.51
1:A:451:LEU:CD1	1:A:452:PRO:HD2	2.30	0.51
1:C:435:VAL:O	1:C:439:VAL:HG23	2.10	0.51
1:B:128:PHE:CD2	1:B:267:ALA:HB1	2.45	0.51
1:D:297:ILE:HD13	1:D:461:VAL:O	2.11	0.51
1:D:470:VAL:HG12	1:D:471:LYS:N	2.26	0.51
1:C:69:MET:HE2	1:C:71:ILE:HD11	1.93	0.51
1:D:334:VAL:HG12	1:D:433:LYS:HE2	1.92	0.51
1:D:158:ASN:HB3	5:D:482:HOH:O	2.10	0.51
1:A:101:VAL:CG1	1:A:102:TYR:HD1	2.24	0.51
1:A:150:ARG:HA	1:A:153:MET:HE2	1.93	0.50
1:B:149:VAL:O	1:B:153:MET:HG3	2.11	0.50
1:B:192:ASP:OD1	1:B:194:ARG:HB2	2.09	0.50
1:B:333:ASN:HA	1:B:337:GLU:HB2	1.93	0.50
1:B:405:MET:HE3	1:B:412:PHE:CD1	2.46	0.50
1:A:350:ARG:C	1:A:350:ARG:HD2	2.32	0.50
1:B:312:LYS:HB2	1:B:313:ARG:NH2	2.26	0.50
1:B:367:GLN:NE2	1:B:367:GLN:N	2.49	0.50
4:C:1:N8E:H013	1:D:45:ILE:HD13	1.90	0.50
3:C:490:TPF:F2	3:C:490:TPF:C5	2.46	0.50
1:A:288:MET:CE	1:A:288:MET:HA	2.41	0.50
1:A:455:ASN:HD22	1:A:455:ASN:C	2.15	0.50
1:B:288:MET:CA	1:B:288:MET:HE2	2.42	0.50
1:B:39:THR:OG1	1:B:43:GLY:O	2.28	0.50
1:A:93:ASN:HA	1:A:96:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ASP:O	1:B:256:ASN:OD1	2.30	0.50
1:B:331:TYR:CE1	1:B:335:MET:CG	2.95	0.50
1:B:406:LYS:O	1:B:406:LYS:CG	2.60	0.50
1:D:82:VAL:CG2	1:D:411:ALA:HA	2.42	0.50
1:A:154:LYS:O	1:A:154:LYS:CG	2.60	0.50
1:C:313:ARG:H	1:C:313:ARG:NE	2.10	0.50
1:D:139:GLN:O	1:D:140:ASN:CG	2.49	0.50
1:D:305:HIS:C	1:D:311:ASN:HD22	2.15	0.50
1:D:406:LYS:O	1:D:407:LEU:C	2.48	0.50
1:B:173:MET:O	1:B:177:THR:HG23	2.11	0.50
1:C:54:GLY:O	1:C:58:LYS:HG3	2.11	0.50
1:C:86:SER:O	1:C:90:THR:HB	2.12	0.50
1:D:293:HIS:HA	1:D:296:THR:HG21	1.94	0.50
1:A:119:TYR:CD1	1:A:120:PRO:CA	2.95	0.50
1:A:142:ALA:HB3	1:A:143:PRO:CD	2.36	0.50
1:A:99:ARG:HG3	1:A:115:TYR:O	2.12	0.50
1:D:192:ASP:C	1:D:192:ASP:OD1	2.50	0.50
1:D:246:ARG:HA	1:D:249:GLU:HG2	1.94	0.50
1:C:156:ASN:HD22	1:C:156:ASN:N	2.06	0.50
1:C:156:ASN:O	1:C:157:TRP:HD1	1.94	0.50
1:A:53:LEU:HG	1:A:57:LEU:HD22	1.94	0.49
1:B:90:THR:HB	1:B:91:PRO:HD3	1.94	0.49
1:A:39:THR:CB	1:C:40:PRO:HG2	2.42	0.49
1:D:139:GLN:O	1:D:140:ASN:OD1	2.30	0.49
1:D:167:LEU:HD13	1:D:300:THR:HG21	1.94	0.49
1:A:135:VAL:HB	1:A:331:TYR:OH	2.12	0.49
1:A:174:ILE:CB	1:A:296:THR:HG22	2.41	0.49
1:B:202:LYS:HB3	1:B:231:ALA:HB2	1.93	0.49
1:C:254:ASP:OD2	1:C:254:ASP:O	2.30	0.49
1:D:404:ASN:HD22	1:D:405:MET:H	1.60	0.49
1:A:206:CYS:O	1:A:208:ILE:CG1	2.60	0.49
1:A:82:VAL:HG23	1:A:85:HIS:CE1	2.47	0.49
1:C:237:ASP:O	1:C:241:GLU:HG3	2.13	0.49
1:A:306:LEU:HD13	1:A:440:LEU:HD11	1.95	0.49
1:C:470:VAL:HG12	1:C:471:LYS:N	2.27	0.49
1:A:235:LEU:CD2	1:A:285:VAL:CG2	2.90	0.49
1:A:39:THR:OG1	1:C:40:PRO:HG2	2.11	0.49
1:B:370:LYS:HE3	1:B:371:TYR:CZ	2.47	0.49
1:D:140:ASN:O	1:D:140:ASN:OD1	2.30	0.49
1:A:192:ASP:OD1	1:A:195:GLN:HG2	2.12	0.49
1:A:50:LYS:HD3	1:A:50:LYS:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:490:TPF:F2	3:B:490:TPF:C5	2.40	0.49
1:C:209:PRO:O	1:C:212:VAL:HG23	2.12	0.49
1:C:271:ASP:OD1	1:C:271:ASP:C	2.49	0.49
1:D:139:GLN:CD	1:D:139:GLN:H	2.13	0.49
1:A:42:VAL:CG2	1:C:40:PRO:CB	2.78	0.49
1:B:416:GLY:N	2:B:481:HEM:HMA3	2.27	0.49
1:A:121:ARG:O	1:A:125:GLN:HG3	2.13	0.49
1:C:246:ARG:HA	1:C:249:GLU:HG2	1.95	0.49
1:C:168:ASP:CG	1:D:194:ARG:NH2	2.66	0.49
1:A:135:VAL:HA	1:A:138:PHE:CE2	2.47	0.48
1:A:455:ASN:ND2	1:A:455:ASN:C	2.66	0.48
1:A:42:VAL:O	1:A:45:ILE:HG22	2.13	0.48
1:B:455:ASN:HD22	1:B:456:TYR:N	2.11	0.48
2:C:481:HEM:HHD	2:C:481:HEM:CBC	2.30	0.48
1:D:220:LEU:HB2	1:D:222:LEU:CD1	2.42	0.48
1:A:53:LEU:CD1	1:A:57:LEU:HD22	2.43	0.48
1:C:182:LEU:CD1	1:C:288:MET:HE1	2.41	0.48
1:D:184:GLY:O	1:D:188:ARG:HG3	2.13	0.48
1:B:105:MET:CE	1:B:109:PHE:HZ	2.26	0.48
1:B:84:GLN:NE2	1:B:369:GLY:HA2	2.29	0.48
1:D:125:GLN:HA	1:D:128:PHE:HD1	1.78	0.48
1:A:157:TRP:NE1	1:A:164:ILE:HD13	2.28	0.48
1:C:95:ILE:HG21	1:C:366:VAL:HG12	1.96	0.48
1:D:106:VAL:N	1:D:107:PRO:HD2	2.29	0.48
1:D:145:ILE:O	1:D:149:VAL:HG23	2.13	0.48
1:D:214:LEU:CB	1:D:217:ILE:HG22	2.42	0.48
1:B:325:PHE:HB3	1:B:329:LEU:CD2	2.43	0.48
1:C:81:ASP:OD2	1:C:84:GLN:HG2	2.13	0.48
1:C:168:ASP:CG	1:D:194:ARG:HH21	2.17	0.48
1:D:214:LEU:HB2	1:D:217:ILE:CG2	2.43	0.48
1:C:200:LEU:HB3	1:C:204:GLU:OE2	2.13	0.48
1:D:82:VAL:HG22	1:D:411:ALA:HA	1.95	0.48
1:C:252:GLN:NE2	1:C:254:ASP:H	2.11	0.48
1:C:289:PHE:CD2	1:C:289:PHE:C	2.87	0.48
1:C:422:CYS:HA	2:C:481:HEM:CHA	2.44	0.48
1:D:350:ARG:C	1:D:350:ARG:CD	2.81	0.48
1:A:202:LYS:HB3	1:A:231:ALA:HB2	1.94	0.48
1:A:94:GLU:O	1:A:363:LEU:HB2	2.14	0.48
1:B:216:TRP:CB	1:C:215:PRO:HG2	2.43	0.48
1:B:381:CYS:O	1:B:383:PRO:HD3	2.12	0.48
1:B:338:MET:HE3	1:B:437:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:HIS:CA	1:D:296:THR:HG22	2.44	0.48
1:A:106:VAL:N	1:A:107:PRO:CD	2.76	0.48
1:A:331:TYR:O	1:A:335:MET:HG2	2.14	0.48
1:A:42:VAL:CG2	1:C:41:PHE:HD2	2.27	0.48
1:B:261:LEU:O	1:B:265:LEU:HG	2.13	0.48
1:C:319:HIS:HA	1:C:322:ILE:HG12	1.95	0.48
1:D:220:LEU:HB2	1:D:222:LEU:HD13	1.96	0.48
1:D:404:ASN:HD22	1:D:405:MET:N	2.12	0.48
3:A:490:TPF:C5	3:A:490:TPF:F2	2.50	0.48
1:D:146:GLN:NE2	1:D:329:LEU:HG	2.29	0.48
1:B:138:PHE:HD1	1:B:141:PHE:CD2	2.31	0.47
1:B:203:MET:HG3	1:B:231:ALA:HB3	1.95	0.47
1:B:213:PHE:C	1:B:215:PRO:HD3	2.35	0.47
1:C:202:LYS:NZ	1:C:202:LYS:HB3	2.29	0.47
1:D:134:THR:C	1:D:138:PHE:CE1	2.87	0.47
1:D:204:GLU:OE1	1:D:289:PHE:CE1	2.67	0.47
1:A:128:PHE:HD1	1:A:275:MET:HE1	1.75	0.47
1:A:240:SER:O	1:A:244:ILE:HG13	2.14	0.47
1:A:324:GLU:O	1:A:324:GLU:HG3	2.15	0.47
1:B:94:GLU:N	1:B:94:GLU:OE1	2.42	0.47
1:A:113:VAL:O	1:A:114:ALA:C	2.50	0.47
1:A:455:ASN:ND2	1:A:457:HIS:H	2.13	0.47
1:B:258:SER:HB3	1:B:262:ALA:CB	2.42	0.47
1:C:106:VAL:HG22	1:C:116:ALA:HB2	1.95	0.47
1:C:297:ILE:HD13	1:C:461:VAL:O	2.14	0.47
1:D:356:VAL:HG12	1:D:357:MET:HG2	1.96	0.47
1:D:432:VAL:O	1:D:436:LEU:HG	2.15	0.47
1:C:106:VAL:HB	1:C:107:PRO:HD3	1.96	0.47
1:C:78:VAL:HA	1:C:380:ALA:O	2.15	0.47
1:A:475:LYS:O	1:A:476:LYS:HB2	2.15	0.47
1:C:288:MET:HE2	1:C:288:MET:HA	1.97	0.47
1:D:317:LYS:O	1:D:320:GLN:HB2	2.15	0.47
1:A:313:ARG:HG2	1:A:314:HIS:N	2.30	0.47
1:B:325:PHE:HE2	1:B:333:ASN:CB	2.26	0.47
1:C:128:PHE:CD1	1:C:275:MET:HE2	2.45	0.47
1:C:42:VAL:CG1	1:C:45:ILE:CG2	2.84	0.47
1:D:172:ALA:O	1:D:175:ILE:HG22	2.14	0.47
1:A:135:VAL:HA	1:A:138:PHE:HD2	1.76	0.47
1:B:141:PHE:O	1:B:145:ILE:HG13	2.15	0.47
1:B:288:MET:HA	1:B:288:MET:CE	2.44	0.47
1:B:42:VAL:O	1:B:45:ILE:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:LYS:O	1:C:253:LYS:CG	2.63	0.47
1:A:356:VAL:HG22	1:A:384:LEU:HD22	1.96	0.47
1:B:128:PHE:O	1:B:132:GLU:HG2	2.15	0.47
1:B:182:LEU:HD12	1:B:288:MET:CE	2.45	0.47
1:B:395:ASN:N	1:B:396:PRO:HD3	2.29	0.47
1:C:195:GLN:HE22	1:D:164:ILE:HA	1.80	0.47
1:C:95:ILE:CD1	1:C:95:ILE:N	2.73	0.47
1:D:222:LEU:O	1:D:226:TYR:CD2	2.68	0.47
1:B:317:LYS:HA	1:B:320:GLN:HE21	1.79	0.47
1:D:119:TYR:N	1:D:120:PRO:HD2	2.31	0.47
1:D:367:GLN:NE2	1:D:367:GLN:H	1.98	0.47
1:D:36:HIS:CD2	1:D:37:GLY:N	2.83	0.47
1:D:350:ARG:O	1:D:387:HIS:HD2	1.98	0.47
1:B:53:LEU:HD11	1:B:388:GLN:HG3	1.98	0.46
1:B:98:PRO:HG3	1:B:420:HIS:CE1	2.50	0.46
1:C:101:VAL:HG11	1:C:359:MET:CB	2.44	0.46
1:C:36:HIS:HD2	1:C:63:TYR:OH	1.97	0.46
1:B:113:VAL:CG1	1:B:114:ALA:N	2.75	0.46
1:B:191:LEU:HD13	1:B:238:ILE:HD13	1.96	0.46
1:B:217:ILE:HG23	1:B:218:LEU:N	2.29	0.46
1:C:206:CYS:HA	1:C:224:GLN:HB3	1.98	0.46
1:D:324:GLU:O	1:D:324:GLU:HG3	2.15	0.46
1:D:333:ASN:O	1:D:338:MET:CG	2.63	0.46
1:A:195:GLN:O	1:A:198:GLN:HB2	2.15	0.46
1:A:356:VAL:CG2	1:A:384:LEU:HD22	2.45	0.46
1:A:87:LYS:HD3	1:A:367:GLN:O	2.15	0.46
1:B:435:VAL:O	1:B:439:VAL:HG23	2.15	0.46
1:C:44:HIS:HD2	1:C:70:ASN:N	1.89	0.46
1:D:89:PHE:O	1:D:418:GLY:HA3	2.16	0.46
1:D:435:VAL:O	1:D:439:VAL:HG23	2.15	0.46
1:A:370:LYS:HE3	1:A:371:TYR:OH	2.15	0.46
1:C:101:VAL:CG1	1:C:359:MET:HE3	2.45	0.46
1:C:213:PHE:C	1:C:214:LEU:HD12	2.35	0.46
1:C:204:GLU:OE1	1:C:293:HIS:NE2	2.48	0.46
1:D:210:ALA:O	1:D:214:LEU:HD23	2.16	0.46
1:A:78:VAL:CG2	1:A:78:VAL:O	2.63	0.46
1:B:472:TYR:C	1:B:472:TYR:CD1	2.89	0.46
1:A:40:PRO:CG	1:C:39:THR:HB	2.45	0.46
1:C:50:LYS:O	1:C:50:LYS:HD3	2.16	0.46
1:B:239:LEU:O	1:B:243:ILE:HG13	2.16	0.46
1:A:315:LEU:HD11	1:A:319:HIS:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:PRO:HG3	1:A:420:HIS:NE2	2.31	0.46
1:B:106:VAL:HG22	1:B:116:ALA:HB2	1.98	0.46
1:C:470:VAL:CG1	1:C:471:LYS:N	2.79	0.46
1:C:84:GLN:OE1	1:C:87:LYS:HG3	2.16	0.46
1:B:133:LEU:HD13	2:B:481:HEM:HAC	1.98	0.45
1:A:112:GLY:O	1:A:117:ALA:HB2	2.16	0.45
1:A:174:ILE:HB	1:A:296:THR:HG22	1.99	0.45
1:A:128:PHE:CD1	1:A:275:MET:HE3	2.48	0.45
1:B:246:ARG:HA	1:B:249:GLU:HG2	1.98	0.45
1:C:103:SER:O	1:C:106:VAL:HG23	2.15	0.45
1:C:204:GLU:OE1	1:C:293:HIS:HE1	1.97	0.45
1:B:335:MET:CA	1:B:335:MET:CE	2.90	0.45
1:C:170:CYS:O	1:C:174:ILE:HG12	2.17	0.45
1:D:161:GLU:HB2	1:D:471:LYS:HE3	1.99	0.45
1:D:293:HIS:CA	1:D:296:THR:CG2	2.92	0.45
1:C:69:MET:CE	1:C:71:ILE:HD11	2.46	0.45
1:B:119:TYR:N	1:B:120:PRO:CD	2.79	0.45
1:C:321:GLU:OE2	1:C:338:MET:HA	2.17	0.45
1:C:322:ILE:HA	1:C:325:PHE:HD1	1.82	0.45
1:C:455:ASN:ND2	1:C:457:HIS:CD2	2.75	0.45
1:D:138:PHE:CE2	1:D:427:PHE:HA	2.52	0.45
1:B:215:PRO:C	1:B:217:ILE:N	2.69	0.45
1:C:224:GLN:N	1:C:224:GLN:OE1	2.41	0.45
1:C:84:GLN:OE1	1:C:87:LYS:HE3	2.17	0.45
1:D:39:THR:OG1	1:D:43:GLY:N	2.50	0.45
1:A:368:VAL:O	1:A:369:GLY:C	2.55	0.45
1:B:211:ALA:HA	1:B:217:ILE:HG21	1.98	0.45
1:C:101:VAL:O	1:C:101:VAL:CG1	2.65	0.45
1:C:236:GLN:HE22	1:C:278:HIS:HA	1.82	0.45
1:C:53:LEU:CD1	1:C:57:LEU:HD13	2.47	0.45
1:D:470:VAL:CG1	1:D:471:LYS:N	2.79	0.45
1:B:188:ARG:CA	1:B:191:LEU:O	2.52	0.45
1:B:216:TRP:HB3	1:C:215:PRO:HG2	1.99	0.45
1:B:87:LYS:CD	1:B:368:VAL:HA	2.47	0.45
1:D:39:THR:OG1	1:D:42:VAL:CG1	2.64	0.45
1:D:46:ILE:HD12	1:D:46:ILE:N	2.32	0.45
1:D:76:ILE:HA	1:D:378:ILE:O	2.17	0.45
1:A:301:TRP:O	1:A:305:HIS:CD2	2.70	0.45
1:A:325:PHE:HB3	1:A:329:LEU:HD21	1.98	0.45
1:C:141:PHE:HB2	5:C:484:HOH:O	2.17	0.44
1:C:95:ILE:CG2	1:C:366:VAL:HG13	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:MET:HE1	1:A:285:VAL:HG13	1.98	0.44
1:A:129:LEU:HD21	1:A:287:ALA:HB2	1.99	0.44
1:B:45:ILE:HG23	1:B:46:ILE:N	2.33	0.44
1:D:324:GLU:HA	1:D:324:GLU:OE1	2.16	0.44
1:D:470:VAL:HG12	1:D:471:LYS:O	2.17	0.44
1:A:301:TRP:NE1	1:A:463:PRO:HD3	2.33	0.44
1:B:182:LEU:CD1	1:B:288:MET:CE	2.95	0.44
1:B:384:LEU:O	1:B:388:GLN:HG2	2.16	0.44
1:C:82:VAL:CG1	1:C:408:VAL:HG11	2.48	0.44
1:D:389:ASP:O	1:D:391:GLU:N	2.51	0.44
1:D:429:LEU:O	1:D:433:LYS:HD3	2.18	0.44
1:C:163:GLU:OE2	1:C:469:ARG:NH2	2.51	0.44
1:C:377:ASP:OD1	1:C:378:ILE:N	2.51	0.44
1:D:305:HIS:HB3	1:D:399:TRP:CE3	2.53	0.44
1:A:42:VAL:HG12	1:A:45:ILE:HG23	1.97	0.44
1:C:321:GLU:OE1	1:C:340:PHE:HB3	2.17	0.44
1:D:120:PRO:O	1:D:124:GLU:HG3	2.18	0.44
1:A:191:LEU:HD21	1:A:196:PHE:CD2	2.37	0.44
1:B:254:ASP:O	1:B:255:THR:C	2.56	0.44
1:B:350:ARG:O	1:B:387:HIS:CD2	2.70	0.44
1:C:312:LYS:H	1:C:313:ARG:HH21	1.64	0.44
1:C:94:GLU:O	1:C:363:LEU:HB2	2.18	0.44
1:C:453:GLU:CG	1:C:454:PRO:HD2	2.36	0.44
1:C:98:PRO:HG3	1:C:420:HIS:CE1	2.52	0.44
1:A:256:ASN:N	1:A:256:ASN:OD1	2.50	0.44
1:B:81:ASP:OD1	1:B:83:HIS:HB2	2.17	0.44
1:C:103:SER:O	1:C:105:MET:N	2.51	0.44
1:C:383:PRO:O	1:C:387:HIS:CD2	2.70	0.44
1:D:214:LEU:CB	1:D:217:ILE:CG2	2.95	0.44
1:A:51:ASP:C	1:A:51:ASP:OD1	2.56	0.44
1:C:313:ARG:HG2	1:C:314:HIS:N	2.32	0.44
1:D:82:VAL:HG21	1:D:411:ALA:CB	2.48	0.44
1:A:210:ALA:C	1:A:212:VAL:N	2.71	0.44
1:A:39:THR:HG1	1:A:42:VAL:HB	1.81	0.44
1:C:247:GLU:O	1:C:250:GLU:HB3	2.17	0.44
1:D:242:ILE:HD13	1:D:242:ILE:HA	1.92	0.44
1:D:90:THR:N	1:D:91:PRO:CD	2.81	0.44
1:A:238:ILE:O	1:A:242:ILE:HG12	2.17	0.43
1:C:194:ARG:CD	1:D:156:ASN:OD1	2.66	0.43
1:A:216:TRP:HB3	1:D:216:TRP:CH2	2.53	0.43
1:D:78:VAL:HA	1:D:380:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:VAL:HG12	1:A:114:ALA:N	2.33	0.43
1:A:213:PHE:C	1:A:215:PRO:HD3	2.39	0.43
1:A:138:PHE:HD1	1:A:430:LEU:CD2	2.24	0.43
1:B:350:ARG:C	1:B:350:ARG:CD	2.85	0.43
1:B:351:ARG:NH1	1:B:352:ASP:OD1	2.49	0.43
1:B:42:VAL:HB	1:B:45:ILE:HG21	1.99	0.43
1:D:256:ASN:N	1:D:256:ASN:OD1	2.51	0.43
1:D:307:MET:CE	1:D:445:PHE:HB3	2.48	0.43
1:B:215:PRO:O	1:B:217:ILE:N	2.51	0.43
1:C:113:VAL:O	1:C:114:ALA:C	2.54	0.43
1:C:224:GLN:O	1:C:227:ARG:HB2	2.18	0.43
1:D:306:LEU:O	1:D:315:LEU:HD22	2.18	0.43
1:D:353:PRO:HA	1:D:354:PRO:HD3	1.91	0.43
1:D:42:VAL:HG22	1:D:45:ILE:HG22	2.00	0.43
1:A:414:GLY:O	2:A:481:HEM:HMA1	2.18	0.43
1:A:45:ILE:O	1:A:46:ILE:C	2.57	0.43
1:C:142:ALA:CB	1:C:143:PRO:CD	2.94	0.43
1:D:109:PHE:O	1:D:232:ARG:NH2	2.50	0.43
1:A:350:ARG:CD	1:A:350:ARG:C	2.87	0.43
1:A:55:PHE:CE2	1:A:69:MET:CE	3.01	0.43
1:B:301:TRP:O	1:B:305:HIS:CD2	2.71	0.43
1:D:390:GLU:O	1:D:394:PRO:HG3	2.18	0.43
1:B:375:GLU:OE2	1:C:119:TYR:CE2	2.71	0.43
1:C:214:LEU:O	1:C:217:ILE:HG13	2.19	0.43
1:C:365:PRO:HA	1:C:373:VAL:O	2.19	0.43
1:C:51:ASP:OD1	1:C:54:GLY:CA	2.66	0.43
1:D:301:TRP:O	1:D:304:LEU:N	2.52	0.43
1:D:453:GLU:CG	1:D:454:PRO:HD2	2.48	0.43
1:D:358:LEU:HD22	2:D:481:HEM:HBA2	1.99	0.43
1:A:154:LYS:HG2	1:A:154:LYS:O	2.18	0.43
1:A:424:GLY:HA3	2:A:481:HEM:C2C	2.53	0.43
1:A:67:PHE:CZ	1:A:78:VAL:HG21	2.53	0.43
1:C:304:LEU:HB3	1:C:451:LEU:HD11	2.01	0.43
1:D:139:GLN:N	1:D:139:GLN:OE1	2.30	0.43
1:D:353:PRO:CG	1:D:384:LEU:HA	2.49	0.43
1:A:40:PRO:HG3	1:C:39:THR:CG2	2.49	0.43
1:C:177:THR:OG1	1:C:431:GLN:NE2	2.52	0.43
1:C:475:LYS:CA	1:C:475:LYS:HE3	2.49	0.43
1:D:292:GLN:O	1:D:296:THR:CG2	2.59	0.43
1:C:325:PHE:CB	1:C:329:LEU:HD21	2.49	0.43
1:D:54:GLY:O	1:D:58:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:VAL:C	1:A:102:TYR:HD1	2.22	0.43
1:A:223:PRO:HG2	1:A:224:GLN:OE1	2.19	0.43
1:A:69:MET:HB3	1:A:69:MET:HE2	1.90	0.43
1:B:86:SER:O	1:B:90:THR:HB	2.19	0.43
1:C:182:LEU:O	1:C:259:ASP:HB2	2.19	0.43
1:C:362:VAL:HG12	1:C:375:GLU:HA	2.00	0.43
1:D:334:VAL:CG1	1:D:338:MET:SD	3.04	0.43
1:D:353:PRO:HG3	1:D:384:LEU:HA	2.00	0.43
1:B:325:PHE:HB3	1:B:329:LEU:HD21	2.01	0.42
1:B:453:GLU:CG	1:B:454:PRO:HD2	2.46	0.42
1:C:350:ARG:C	1:C:350:ARG:CD	2.88	0.42
1:A:476:LYS:O	1:A:476:LYS:HD3	2.19	0.42
1:A:50:LYS:CD	1:A:50:LYS:C	2.88	0.42
1:B:105:MET:HE1	1:B:109:PHE:HZ	1.84	0.42
1:D:389:ASP:O	1:D:390:GLU:C	2.57	0.42
1:D:60:LYS:HE3	1:D:80:GLY:O	2.19	0.42
2:A:481:HEM:NC	3:A:490:TPF:HC7	2.35	0.42
1:B:101:VAL:HG12	1:B:102:TYR:CE1	2.51	0.42
1:B:213:PHE:C	1:B:214:LEU:CD1	2.88	0.42
1:B:304:LEU:CD1	1:B:452:PRO:HG2	2.47	0.42
1:D:42:VAL:HG22	1:D:45:ILE:HG21	2.01	0.42
1:A:412:PHE:C	1:A:412:PHE:CD2	2.92	0.42
1:B:217:ILE:CG2	1:B:218:LEU:N	2.83	0.42
1:B:271:ASP:C	1:B:271:ASP:OD1	2.57	0.42
1:B:446:GLU:O	1:B:470:VAL:HG13	2.20	0.42
1:C:101:VAL:C	1:C:102:TYR:HD1	2.23	0.42
1:C:103:SER:C	1:C:105:MET:H	2.22	0.42
1:C:105:MET:C	1:C:107:PRO:HD2	2.39	0.42
1:D:179:CYS:HG	1:D:183:PHE:HE1	1.67	0.42
1:D:38:THR:HA	1:D:44:HIS:CE1	2.55	0.42
1:B:220:LEU:O	1:B:222:LEU:N	2.52	0.42
1:B:335:MET:HE3	1:B:335:MET:CA	2.43	0.42
1:C:103:SER:C	1:C:105:MET:N	2.72	0.42
1:C:194:ARG:HD2	1:D:156:ASN:OD1	2.20	0.42
1:C:252:GLN:NE2	1:C:254:ASP:N	2.67	0.42
3:D:490:TPF:C5	3:D:490:TPF:F2	2.48	0.42
1:B:142:ALA:N	1:B:143:PRO:CD	2.82	0.42
1:B:65:GLY:O	1:B:80:GLY:CA	2.67	0.42
1:C:190:ARG:HH22	1:C:241:GLU:CD	2.22	0.42
1:D:82:VAL:HA	1:D:85:HIS:CD2	2.54	0.42
1:A:415:PHE:CZ	1:A:425:GLU:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PHE:HE1	1:A:430:LEU:HD23	1.81	0.42
1:B:330:ASN:N	1:B:333:ASN:ND2	2.32	0.42
1:B:442:ASP:O	1:B:475:LYS:HB2	2.20	0.42
1:C:160:ASP:N	1:C:160:ASP:OD2	2.53	0.42
1:D:325:PHE:HB3	1:D:329:LEU:HD21	2.02	0.42
1:A:160:ASP:N	1:A:160:ASP:OD2	2.52	0.42
1:A:233:ALA:O	1:A:236:GLN:HB3	2.20	0.42
1:B:293:HIS:O	1:B:296:THR:HG23	2.20	0.42
1:C:120:PRO:O	1:C:124:GLU:HG3	2.20	0.42
1:C:166:ILE:HG23	1:C:167:LEU:N	2.35	0.42
1:D:128:PHE:O	1:D:132:GLU:HG2	2.19	0.42
1:D:356:VAL:HG13	1:D:384:LEU:CD2	2.49	0.42
1:D:67:PHE:CZ	1:D:78:VAL:CG2	3.00	0.42
1:B:254:ASP:O	1:B:256:ASN:CG	2.58	0.42
1:B:268:VAL:HG12	1:B:269:TYR:O	2.20	0.42
1:C:124:GLU:OE2	1:C:269:TYR:HD2	2.03	0.42
1:D:301:TRP:O	1:D:302:SER:C	2.58	0.42
1:D:61:LYS:HB3	1:D:61:LYS:NZ	2.35	0.42
1:D:82:VAL:CG2	1:D:411:ALA:CB	2.98	0.42
1:D:86:SER:O	1:D:90:THR:HB	2.20	0.42
1:B:100:GLU:CD	1:B:100:GLU:H	2.22	0.41
1:B:324:GLU:OE1	1:B:324:GLU:HA	2.19	0.41
1:B:82:VAL:HA	1:B:85:HIS:CD2	2.54	0.41
1:C:196:PHE:C	1:C:198:GLN:N	2.74	0.41
1:C:334:VAL:HA	1:C:338:MET:SD	2.60	0.41
1:D:293:HIS:O	1:D:296:THR:CG2	2.67	0.41
1:D:90:THR:HB	1:D:91:PRO:HD3	2.01	0.41
1:C:387:HIS:CE1	1:C:412:PHE:HA	2.55	0.41
1:D:206:CYS:SG	1:D:225:SER:HA	2.60	0.41
1:D:358:LEU:HD22	2:D:481:HEM:CBA	2.50	0.41
1:C:89:PHE:CD2	1:C:417:ALA:HB3	2.55	0.41
1:C:452:PRO:CA	1:C:467:GLN:OE1	2.67	0.41
1:D:101:VAL:HG11	1:D:359:MET:CB	2.50	0.41
1:D:113:VAL:H	1:D:116:ALA:HB3	1.85	0.41
1:A:120:PRO:CG	1:A:121:ARG:H	2.33	0.41
1:A:288:MET:HE2	1:A:288:MET:N	2.35	0.41
1:A:46:ILE:HG22	1:A:47:GLN:N	2.35	0.41
1:C:67:PHE:CE2	1:C:78:VAL:CG2	3.03	0.41
1:D:331:TYR:CZ	1:D:335:MET:HG3	2.55	0.41
1:A:172:ALA:O	1:A:175:ILE:HG22	2.21	0.41
1:A:261:LEU:O	1:A:265:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ASN:O	1:A:403:ARG:HG2	2.20	0.41
1:D:312:LYS:N	1:D:313:ARG:HH21	2.17	0.41
1:D:415:PHE:CE2	1:D:425:GLU:HG3	2.55	0.41
1:A:142:ALA:CB	1:A:143:PRO:HD3	2.36	0.41
1:A:128:PHE:CD1	1:A:275:MET:CE	2.94	0.41
1:C:246:ARG:O	1:C:250:GLU:N	2.54	0.41
1:D:217:ILE:HG21	1:D:217:ILE:HD13	1.78	0.41
1:B:157:TRP:HB3	1:B:472:TYR:CZ	2.56	0.41
1:C:202:LYS:HZ3	1:C:202:LYS:HB3	1.86	0.41
1:C:418:GLY:O	1:C:421:LYS:HG2	2.21	0.41
1:C:457:HIS:CE1	1:D:230:ASP:OD2	2.73	0.41
1:B:145:ILE:O	1:B:149:VAL:HG23	2.21	0.41
1:C:113:VAL:CG1	1:C:114:ALA:N	2.84	0.41
1:D:375:GLU:OE1	1:D:375:GLU:N	2.37	0.41
1:A:139:GLN:OE1	1:A:140:ASN:CG	2.59	0.41
1:D:125:GLN:HG2	1:D:275:MET:HE3	2.02	0.41
1:D:334:VAL:HG22	1:D:338:MET:SD	2.61	0.41
1:D:350:ARG:HA	1:D:387:HIS:HD2	1.80	0.41
1:D:473:ILE:CD1	1:D:473:ILE:N	2.83	0.41
1:A:48:PHE:CD1	1:A:69:MET:HE1	2.52	0.41
1:A:52:PRO:O	1:A:56:MET:HG3	2.21	0.41
1:B:95:ILE:H	1:B:95:ILE:CD1	2.34	0.41
1:C:192:ASP:C	1:C:192:ASP:OD1	2.59	0.41
1:C:240:SER:C	1:C:244:ILE:HD11	2.41	0.41
1:C:308:ASP:OD1	1:C:309:PRO:N	2.54	0.41
1:D:207:LEU:O	1:D:209:PRO:HD3	2.21	0.41
1:A:100:GLU:H	1:A:100:GLU:CD	2.24	0.41
1:A:235:LEU:HD21	1:A:285:VAL:HG22	2.00	0.41
1:A:395:ASN:N	1:A:396:PRO:HD3	2.36	0.41
1:B:45:ILE:HG23	1:B:46:ILE:CD1	2.50	0.41
1:C:156:ASN:C	1:C:157:TRP:CD1	2.94	0.41
1:C:175:ILE:HD12	1:C:175:ILE:HA	1.92	0.41
1:C:415:PHE:CZ	1:C:425:GLU:HG3	2.56	0.41
1:D:105:MET:C	1:D:107:PRO:HD2	2.41	0.41
1:A:138:PHE:CD1	1:A:141:PHE:CD2	3.10	0.40
1:A:174:ILE:HG13	1:A:296:THR:HG22	2.03	0.40
1:A:40:PRO:HG2	1:A:41:PHE:H	1.86	0.40
1:D:333:ASN:O	1:D:338:MET:HG2	2.20	0.40
1:D:298:THR:HG23	1:D:349:ILE:HG13	2.03	0.40
1:C:139:GLN:OE1	1:C:139:GLN:HA	2.22	0.40
1:C:76:ILE:HA	1:C:378:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:VAL:CG2	1:B:461:VAL:HG21	2.49	0.40
1:C:113:VAL:HG12	1:C:114:ALA:N	2.35	0.40
1:C:453:GLU:HG3	1:C:454:PRO:CD	2.42	0.40
1:A:453:GLU:CG	1:A:454:PRO:HD2	2.48	0.40
1:A:90:THR:N	1:A:91:PRO:CD	2.85	0.40
1:B:219:LYS:HE2	1:C:73:GLY:O	2.21	0.40
1:D:214:LEU:HB2	1:D:217:ILE:HG21	2.04	0.40
1:D:404:ASN:OD1	1:D:406:LYS:HG2	2.21	0.40
1:D:69:MET:HE2	1:D:69:MET:HB3	1.98	0.40
1:A:381:CYS:O	1:A:383:PRO:HD3	2.22	0.40
1:B:214:LEU:CD1	1:B:214:LEU:N	2.84	0.40
1:B:365:PRO:HD3	1:B:375:GLU:OE1	2.22	0.40
1:C:157:TRP:NE1	1:C:164:ILE:HD13	2.37	0.40
1:C:76:ILE:HD11	1:C:357:MET:HE1	2.03	0.40
1:C:427:PHE:O	1:C:430:LEU:HB3	2.22	0.40
1:C:45:ILE:HG23	1:C:46:ILE:CD1	2.52	0.40
1:D:131:GLU:O	1:D:137:LYS:HE3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	446/453 (98%)	428 (96%)	18 (4%)	0	100	100
1	B	447/453 (99%)	422 (94%)	24 (5%)	1 (0%)	47	69
1	C	443/453 (98%)	419 (95%)	24 (5%)	0	100	100
1	D	441/453 (97%)	420 (95%)	21 (5%)	0	100	100
All	All	1777/1812 (98%)	1689 (95%)	87 (5%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	339	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	386/388 (100%)	370 (96%)	16 (4%)	30	50
1	B	387/388 (100%)	370 (96%)	17 (4%)	28	47
1	C	385/388 (99%)	372 (97%)	13 (3%)	37	58
1	D	383/388 (99%)	369 (96%)	14 (4%)	34	54
All	All	1541/1552 (99%)	1481 (96%)	60 (4%)	32	52

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	38	THR
1	A	45	ILE
1	A	57	LEU
1	A	78	VAL
1	A	119	TYR
1	A	160	ASP
1	A	206	CYS
1	A	258	SER
1	A	313	ARG
1	A	367	GLN
1	A	395	ASN
1	A	406	LYS
1	A	413	CYS
1	A	455	ASN
1	A	476	LYS
1	B	39	THR
1	B	57	LEU
1	B	76	ILE
1	B	95	ILE
1	B	194	ARG

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Mol	Chain	Res	Type
1	B	214	LEU
1	B	254	ASP
1	B	296	THR
1	B	313	ARG
1	B	330	ASN
1	B	333	ASN
1	B	367	GLN
1	B	387	HIS
1	B	395	ASN
1	B	406	LYS
1	B	455	ASN
1	B	475	LYS
1	C	35	VAL
1	C	57	LEU
1	C	81	ASP
1	C	82	VAL
1	C	156	ASN
1	C	160	ASP
1	C	244	ILE
1	C	252	GLN
1	C	296	THR
1	C	313	ARG
1	C	458	THR
1	C	475	LYS
1	C	476	LYS
1	D	28	LYS
1	D	61	LYS
1	D	76	ILE
1	D	160	ASP
1	D	192	ASP
1	D	214	LEU
1	D	217	ILE
1	D	313	ARG
1	D	367	GLN
1	D	387	HIS
1	D	388	GLN
1	D	404	ASN
1	D	407	LEU
1	D	413	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	44	HIS
1	A	156	ASN
1	A	198	GLN
1	A	278	HIS
1	A	320	GLN
1	A	367	GLN
1	A	387	HIS
1	A	395	ASN
1	A	431	GLN
1	A	455	ASN
1	B	44	HIS
1	B	139	GLN
1	B	278	HIS
1	B	305	HIS
1	B	314	HIS
1	B	320	GLN
1	B	328	GLN
1	B	330	ASN
1	B	333	ASN
1	B	367	GLN
1	B	387	HIS
1	B	431	GLN
1	B	455	ASN
1	C	36	HIS
1	C	44	HIS
1	C	156	ASN
1	C	278	HIS
1	C	293	HIS
1	C	314	HIS
1	C	320	GLN
1	C	387	HIS
1	C	431	GLN
1	C	455	ASN
1	C	457	HIS
1	D	36	HIS
1	D	44	HIS
1	D	198	GLN
1	D	256	ASN
1	D	278	HIS
1	D	320	GLN
1	D	328	GLN
1	D	333	ASN

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Mol	Chain	Res	Type
1	D	367	GLN
1	D	387	HIS
1	D	388	GLN
1	D	431	GLN
1	D	455	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	HEM	A	481	1,3	27,50,50	2.21	6 (22%)	17,82,82	1.32	2 (11%)
2	HEM	B	481	1,3	27,50,50	2.17	5 (18%)	17,82,82	1.40	2 (11%)
3	TPF	A	490	2	18,24,24	4.50	5 (27%)	24,34,34	2.78	10 (41%)
3	TPF	C	490	2	18,24,24	4.45	5 (27%)	24,34,34	2.89	10 (41%)
4	N8E	C	1	-	23,23,23	0.42	0	22,22,22	0.40	0
2	HEM	D	481	1,3	27,50,50	2.19	5 (18%)	17,82,82	1.45	3 (17%)
3	TPF	B	490	2	18,24,24	4.48	5 (27%)	24,34,34	2.90	11 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TPF	D	490	2	18,24,24	4.43	5 (27%)	24,34,34	2.88	11 (45%)
2	HEM	C	481	1,3	27,50,50	2.20	6 (22%)	17,82,82	1.47	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	481	1,3	-	0/6/54/54	-
2	HEM	B	481	1,3	-	0/6/54/54	-
3	TPF	A	490	2	-	6/16/16/16	0/3/3/3
3	TPF	C	490	2	-	6/16/16/16	0/3/3/3
4	N8E	C	1	-	-	8/21/21/21	-
2	HEM	D	481	1,3	-	0/6/54/54	-
3	TPF	B	490	2	-	9/16/16/16	0/3/3/3
3	TPF	D	490	2	-	6/16/16/16	0/3/3/3
2	HEM	C	481	1,3	-	0/6/54/54	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	490	TPF	C6-N4	13.21	1.46	1.33
3	B	490	TPF	C6-N4	13.16	1.46	1.33
3	C	490	TPF	C6-N4	12.84	1.46	1.33
3	D	490	TPF	C6-N4	12.82	1.46	1.33
3	C	490	TPF	C3-N1	12.02	1.45	1.33
3	A	490	TPF	C3-N1	11.92	1.45	1.33
3	D	490	TPF	C3-N1	11.88	1.45	1.33
3	B	490	TPF	C3-N1	11.78	1.45	1.33
2	B	481	HEM	C3D-C2D	5.47	1.53	1.37
2	D	481	HEM	C3D-C2D	5.45	1.53	1.37
2	A	481	HEM	C3D-C2D	5.43	1.53	1.37
2	C	481	HEM	C3D-C2D	5.32	1.53	1.37
2	A	481	HEM	C3C-C2C	-4.76	1.33	1.40
2	C	481	HEM	C3B-C2B	-4.69	1.33	1.40
2	D	481	HEM	C3B-C2B	-4.67	1.33	1.40
2	D	481	HEM	C3C-C2C	-4.66	1.33	1.40
2	C	481	HEM	C3C-C2C	-4.60	1.34	1.40
2	B	481	HEM	C3C-C2C	-4.60	1.34	1.40
2	A	481	HEM	C3B-C2B	-4.58	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	481	HEM	C3B-C2B	-4.47	1.34	1.40
3	A	490	TPF	N3-N1	4.40	1.41	1.35
3	C	490	TPF	N3-N1	4.36	1.41	1.35
3	B	490	TPF	N6-N4	4.26	1.41	1.35
3	B	490	TPF	N3-N1	4.26	1.41	1.35
3	D	490	TPF	N3-N1	4.25	1.41	1.35
3	C	490	TPF	N6-N4	4.23	1.41	1.35
3	D	490	TPF	N6-N4	4.16	1.41	1.35
3	A	490	TPF	N6-N4	4.06	1.41	1.35
2	C	481	HEM	C3C-CAC	3.50	1.55	1.47
2	D	481	HEM	C3C-CAC	3.44	1.54	1.47
2	C	481	HEM	C3B-CAB	3.41	1.54	1.47
2	B	481	HEM	C3B-CAB	3.37	1.54	1.47
2	B	481	HEM	C3C-CAC	3.36	1.54	1.47
2	D	481	HEM	C3B-CAB	3.33	1.54	1.47
2	A	481	HEM	C3B-CAB	3.29	1.54	1.47
2	A	481	HEM	C3C-CAC	3.22	1.54	1.47
3	D	490	TPF	C1-C8	-2.78	1.50	1.53
3	B	490	TPF	C1-C8	-2.62	1.50	1.53
3	A	490	TPF	C1-C8	-2.49	1.50	1.53
3	C	490	TPF	C1-C8	-2.22	1.50	1.53
2	C	481	HEM	CAA-C2A	2.07	1.55	1.52
2	A	481	HEM	CAA-C2A	2.04	1.55	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	490	TPF	C3-N2-C4	6.97	110.19	102.34
3	C	490	TPF	C3-N2-C4	6.95	110.17	102.34
3	A	490	TPF	C3-N2-C4	6.81	110.01	102.34
3	D	490	TPF	C3-N2-C4	6.79	109.99	102.34
3	C	490	TPF	C6-N5-C7	5.64	108.70	102.34
3	C	490	TPF	N2-C3-N1	-5.26	105.88	112.24
3	B	490	TPF	N2-C3-N1	-5.22	105.93	112.24
3	D	490	TPF	N2-C3-N1	-5.19	105.97	112.24
3	D	490	TPF	C6-N5-C7	5.17	108.16	102.34
3	A	490	TPF	N2-C3-N1	-5.05	106.14	112.24
3	B	490	TPF	C1-C8-C13	-5.02	118.70	122.84
3	D	490	TPF	C1-C8-C13	-4.99	118.73	122.84
3	A	490	TPF	C6-N5-C7	4.95	107.92	102.34
3	B	490	TPF	C6-N5-C7	4.86	107.82	102.34
3	C	490	TPF	C1-C8-C13	-4.41	119.21	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	490	TPF	N5-C6-N4	-4.39	106.93	112.24
3	A	490	TPF	N5-C6-N4	-3.94	107.48	112.24
3	D	490	TPF	N5-C6-N4	-3.88	107.55	112.24
3	B	490	TPF	N5-C6-N4	-3.68	107.79	112.24
3	A	490	TPF	C1-C8-C13	-3.52	119.94	122.84
3	A	490	TPF	C12-C13-C8	-3.48	120.22	124.00
3	D	490	TPF	C12-C13-C8	-3.47	120.24	124.00
3	D	490	TPF	C9-C8-C13	3.44	120.37	116.10
3	B	490	TPF	C12-C13-C8	-3.40	120.31	124.00
3	B	490	TPF	C9-C8-C13	3.39	120.31	116.10
3	A	490	TPF	C9-C8-C13	3.30	120.20	116.10
3	C	490	TPF	C12-C13-C8	-3.24	120.48	124.00
2	C	481	HEM	CAD-CBD-CGD	-3.07	107.52	112.67
3	C	490	TPF	C9-C8-C13	3.01	119.84	116.10
3	C	490	TPF	C13-C12-C11	3.01	119.78	116.62
3	B	490	TPF	C13-C12-C11	2.86	119.62	116.62
3	D	490	TPF	C13-C12-C11	2.84	119.61	116.62
3	A	490	TPF	C13-C12-C11	2.82	119.58	116.62
2	D	481	HEM	CAD-CBD-CGD	-2.71	108.13	112.67
2	D	481	HEM	C1D-C2D-C3D	-2.58	105.20	107.00
3	C	490	TPF	C10-C11-C12	-2.55	119.97	123.29
2	A	481	HEM	CBA-CAA-C2A	-2.46	107.94	112.49
3	B	490	TPF	C10-C11-C12	-2.46	120.09	123.29
2	B	481	HEM	CBA-CAA-C2A	-2.42	108.02	112.49
3	D	490	TPF	C10-C11-C12	-2.42	120.15	123.29
3	B	490	TPF	C6-N4-N6	-2.42	105.34	109.01
3	A	490	TPF	C10-C11-C12	-2.41	120.16	123.29
2	C	481	HEM	C1D-C2D-C3D	-2.39	105.33	107.00
2	D	481	HEM	CBA-CAA-C2A	-2.35	108.14	112.49
3	A	490	TPF	C5-C1-C8	-2.29	105.17	110.87
3	D	490	TPF	C6-N4-N6	-2.28	105.55	109.01
3	D	490	TPF	C5-C1-C8	-2.27	105.22	110.87
2	A	481	HEM	C4C-C3C-C2C	2.27	108.48	106.90
2	C	481	HEM	CBA-CAA-C2A	-2.23	108.37	112.49
3	C	490	TPF	C5-C1-C8	-2.13	105.56	110.87
2	B	481	HEM	C1D-C2D-C3D	-2.11	105.53	107.00
3	B	490	TPF	C5-C1-C8	-2.03	105.80	110.87

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	490	TPF	O-C1-C5-N4
3	A	490	TPF	C2-C1-C5-N4
3	A	490	TPF	C8-C1-C5-N4
3	A	490	TPF	C1-C2-N1-C3
3	A	490	TPF	C1-C5-N4-C6
3	C	490	TPF	O-C1-C5-N4
3	C	490	TPF	C2-C1-C5-N4
3	C	490	TPF	C8-C1-C5-N4
3	C	490	TPF	C1-C5-N4-C6
3	B	490	TPF	O-C1-C5-N4
3	B	490	TPF	C8-C1-C5-N4
3	B	490	TPF	C1-C2-N1-C3
3	B	490	TPF	C1-C5-N4-C6
3	D	490	TPF	O-C1-C5-N4
3	D	490	TPF	C8-C1-C5-N4
3	D	490	TPF	C1-C2-N1-C3
3	D	490	TPF	C1-C5-N4-C6
4	C	1	N8E	C11-C10-O09-C08
3	B	490	TPF	C2-C1-C5-N4
3	D	490	TPF	C2-C1-C5-N4
4	C	1	N8E	O15-C16-C17-O18
4	C	1	N8E	C04-C05-C06-C07
4	C	1	N8E	C23-C22-O21-C20
4	C	1	N8E	O12-C13-C14-O15
3	B	490	TPF	O-C1-C8-C13
3	B	490	TPF	C1-C5-N4-N6
3	D	490	TPF	C1-C5-N4-N6
4	C	1	N8E	O21-C22-C23-O24
3	B	490	TPF	C2-C1-C8-C13
3	B	490	TPF	C5-C1-C8-C13
4	C	1	N8E	C02-C03-C04-C05
4	C	1	N8E	O09-C10-C11-O12
3	A	490	TPF	C1-C5-N4-N6
3	C	490	TPF	C1-C5-N4-N6
3	C	490	TPF	O-C1-C8-C13

There are no ring outliers.

9 monomers are involved in 54 short contacts:

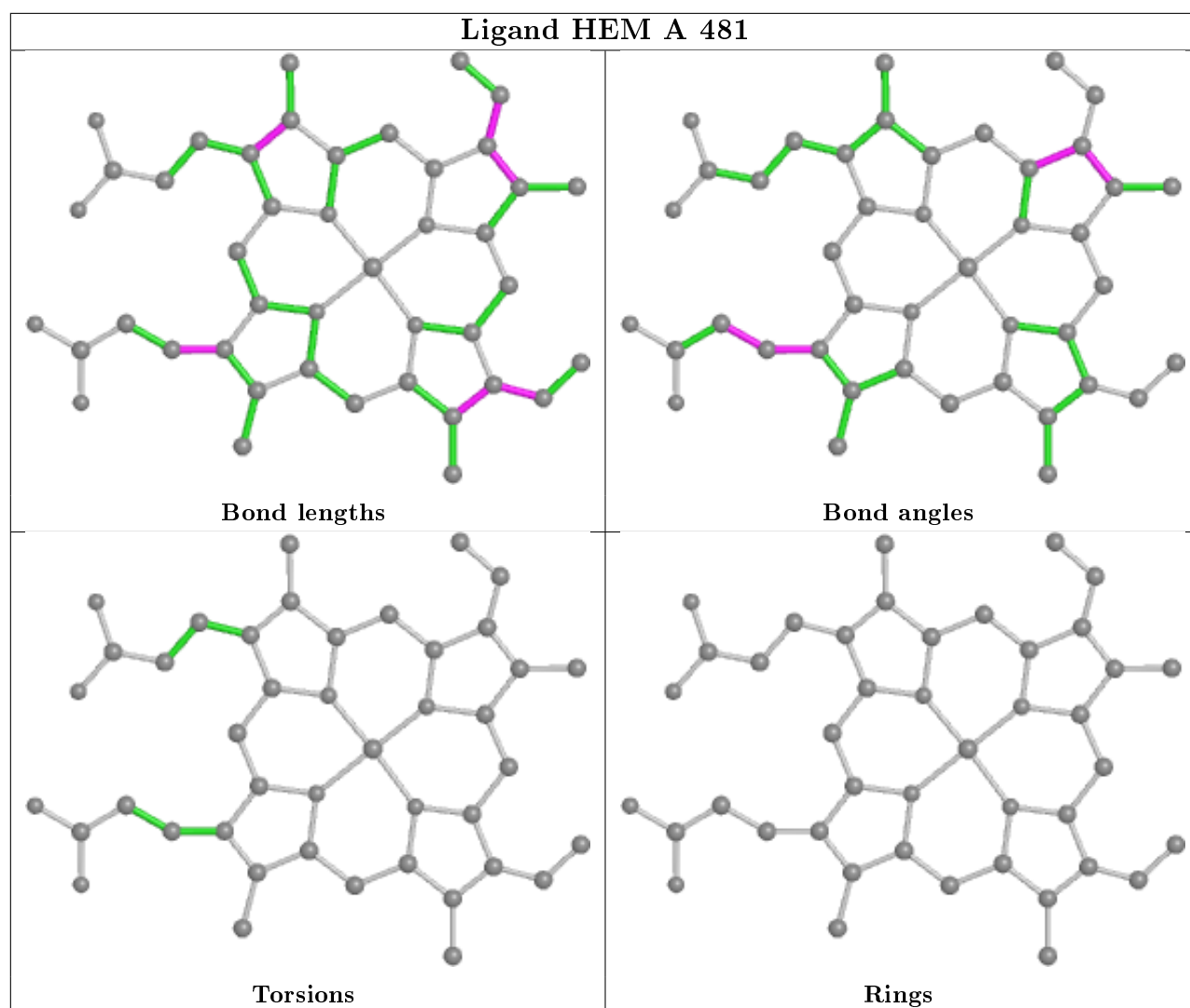
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	481	HEM	6	0
2	B	481	HEM	4	0
3	A	490	TPF	6	0

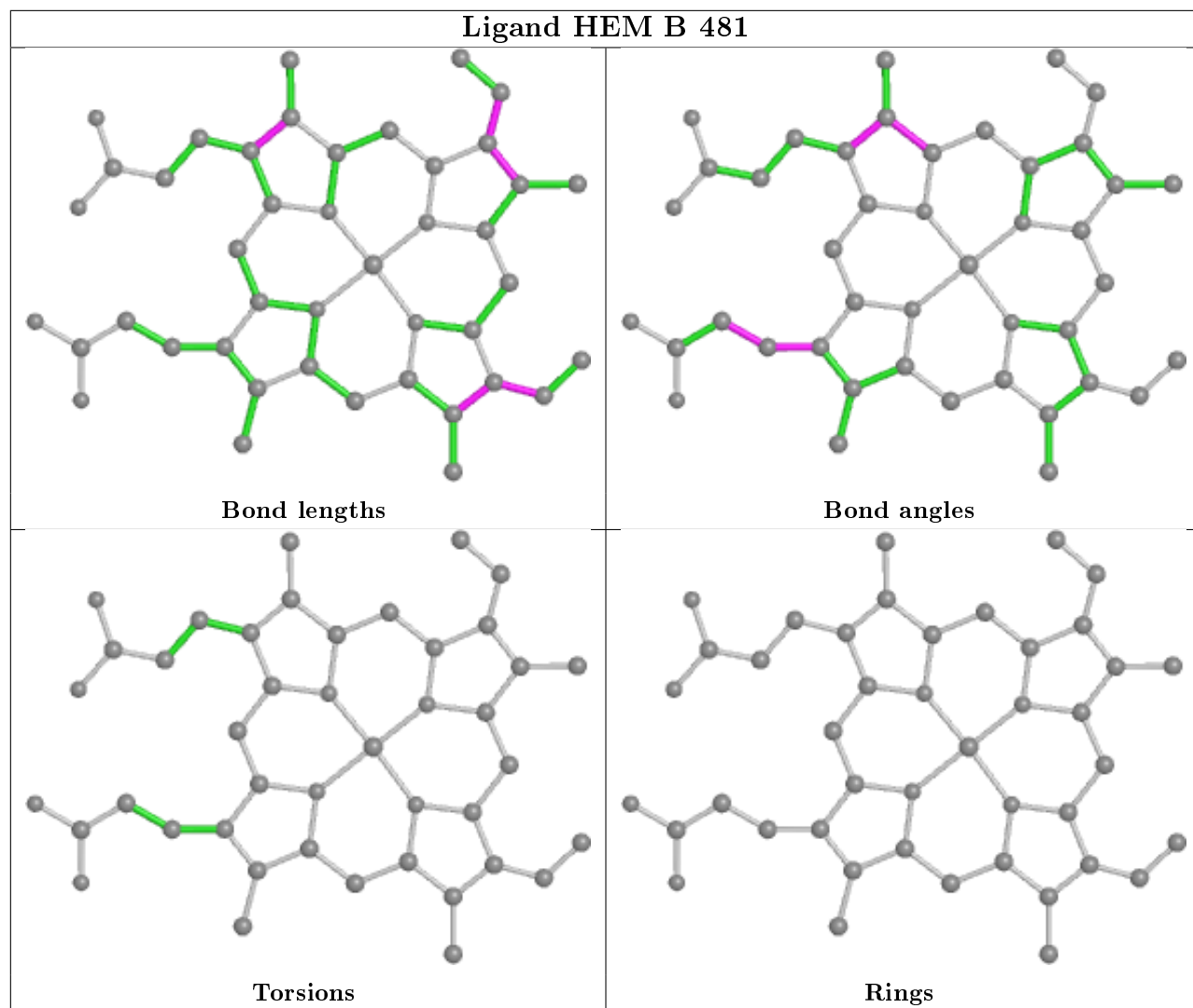
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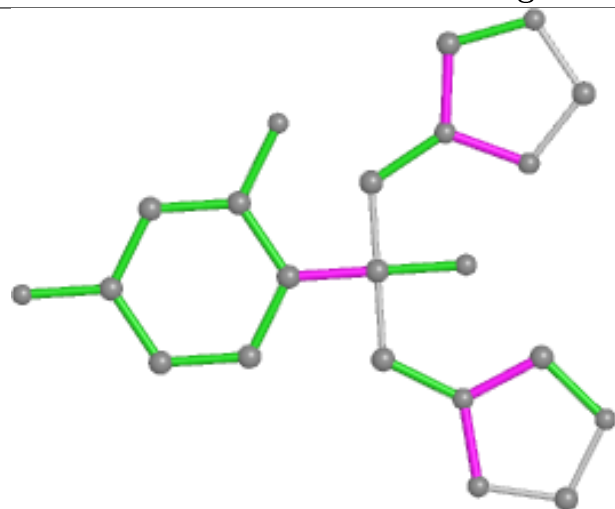
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	490	TPF	6	0
4	C	1	N8E	8	0
2	D	481	HEM	8	0
3	B	490	TPF	6	0
3	D	490	TPF	4	0
2	C	481	HEM	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

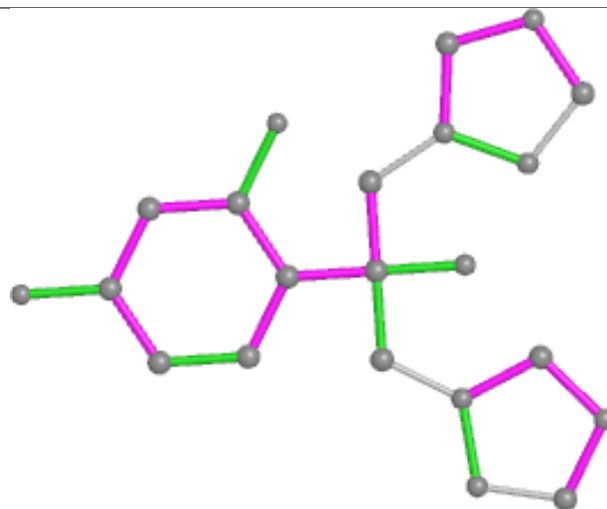




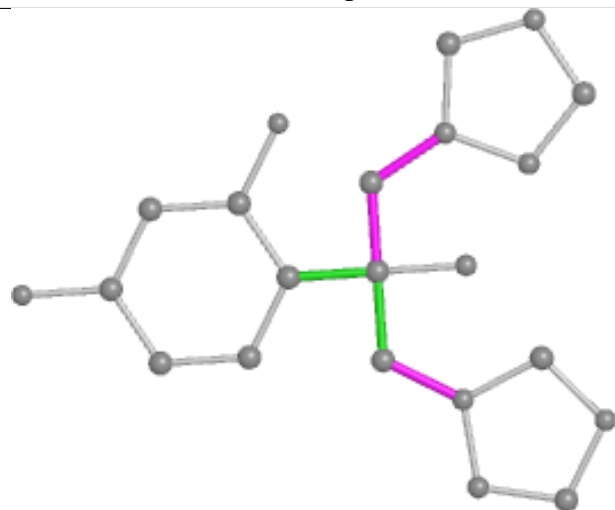
Ligand TPF A 490



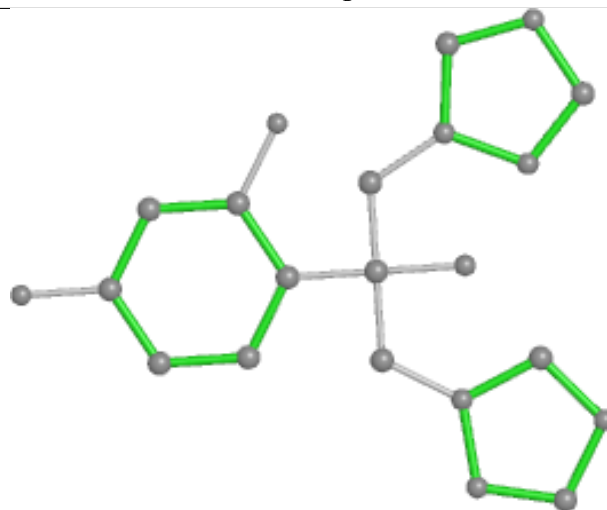
Bond lengths



Bond angles

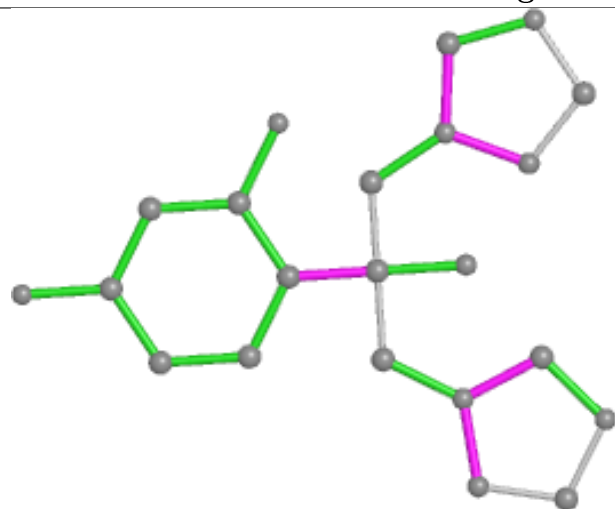


Torsions

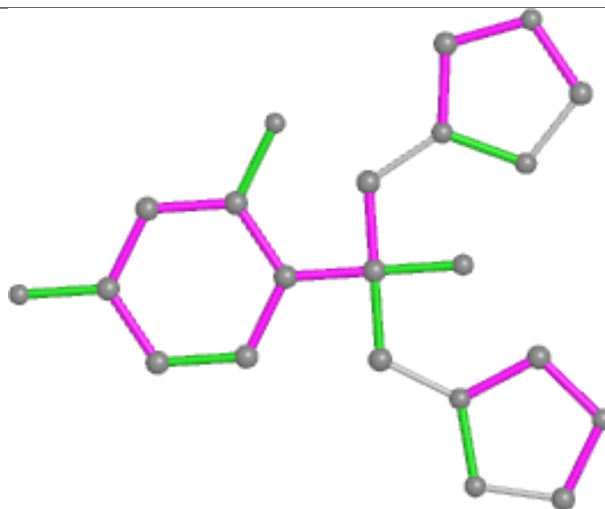


Rings

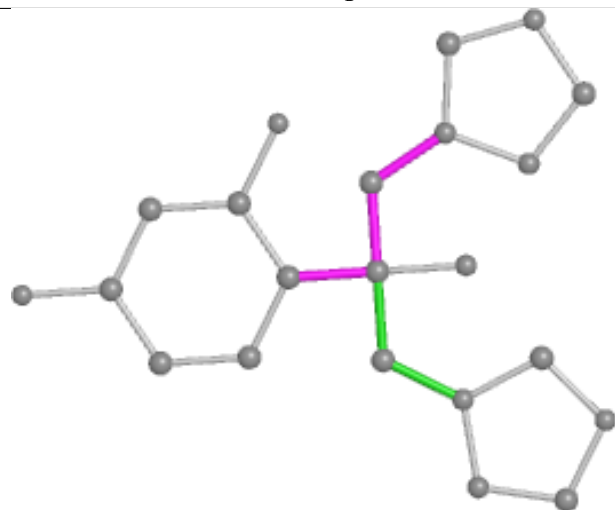
Ligand TPF C 490



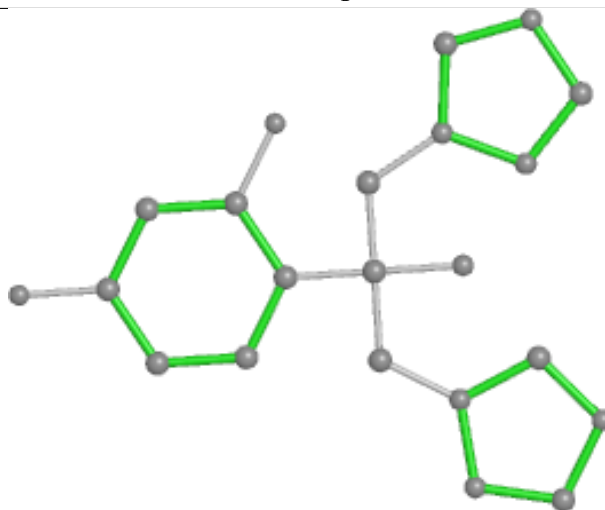
Bond lengths



Bond angles



Torsions



Rings

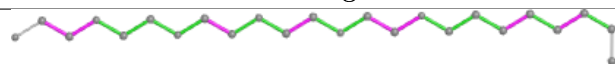
Ligand N8E C 1



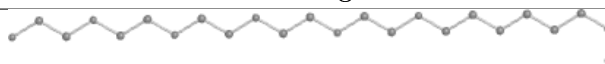
Bond lengths



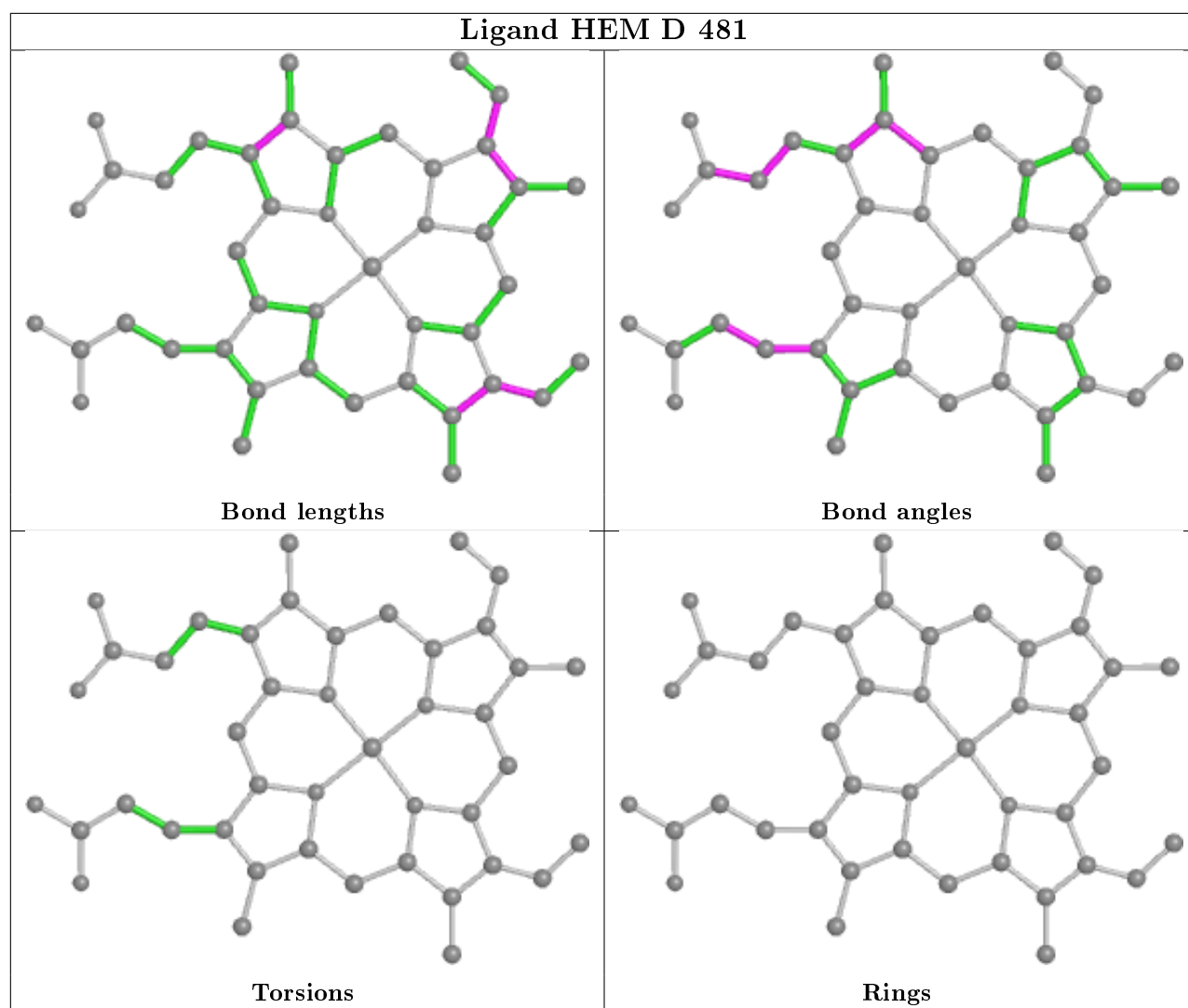
Bond angles



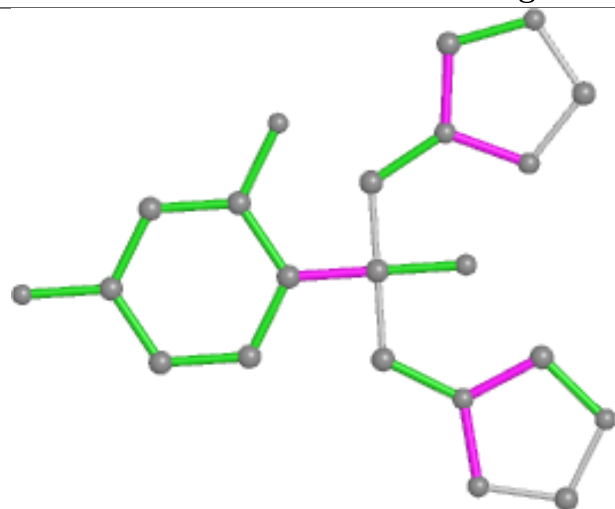
Torsions



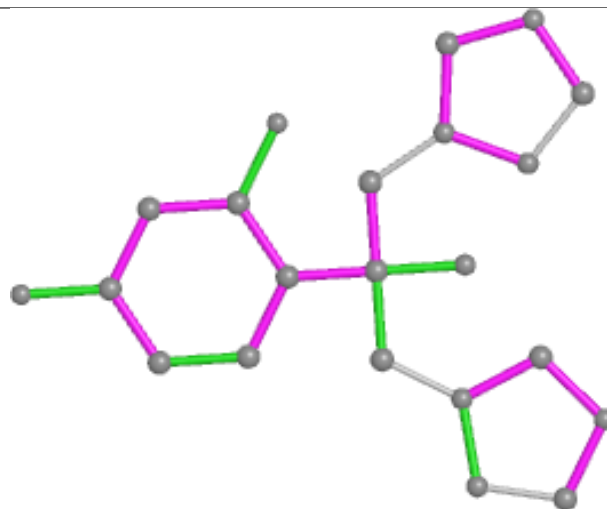
Rings



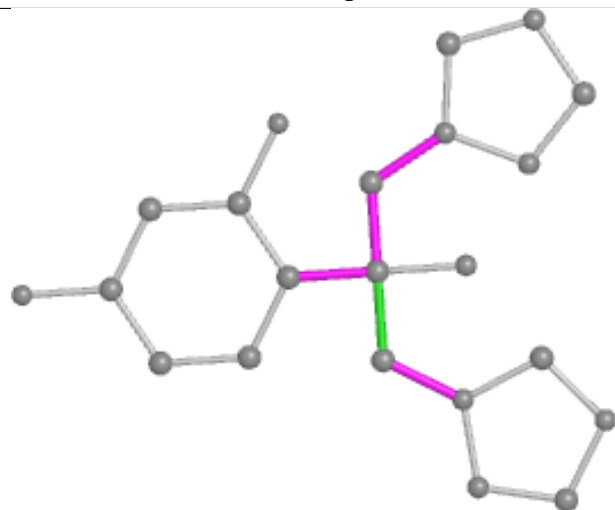
Ligand TPF B 490



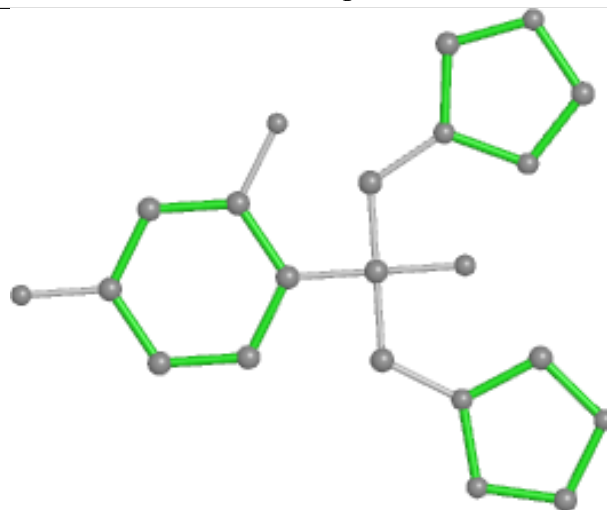
Bond lengths



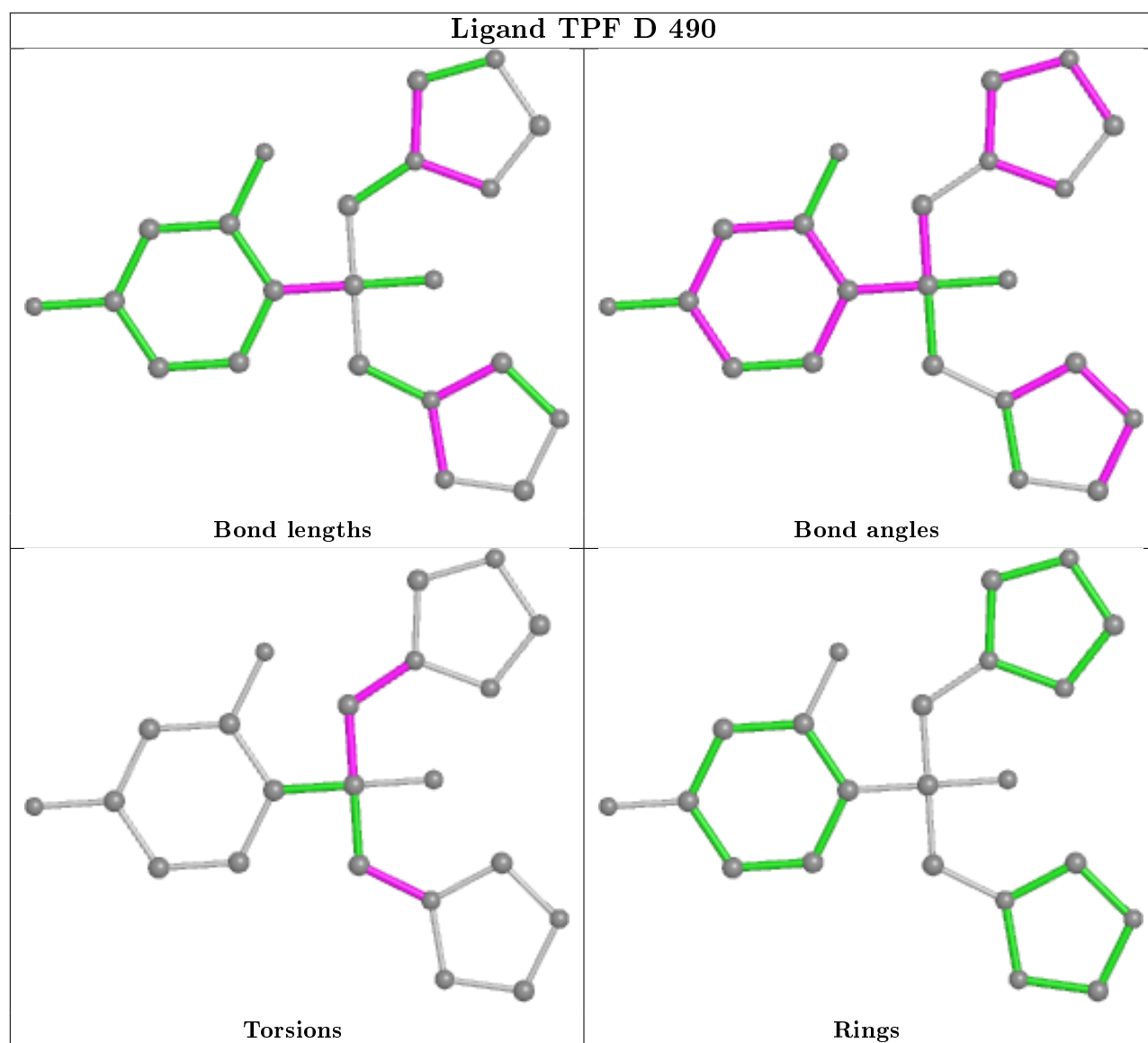
Bond angles

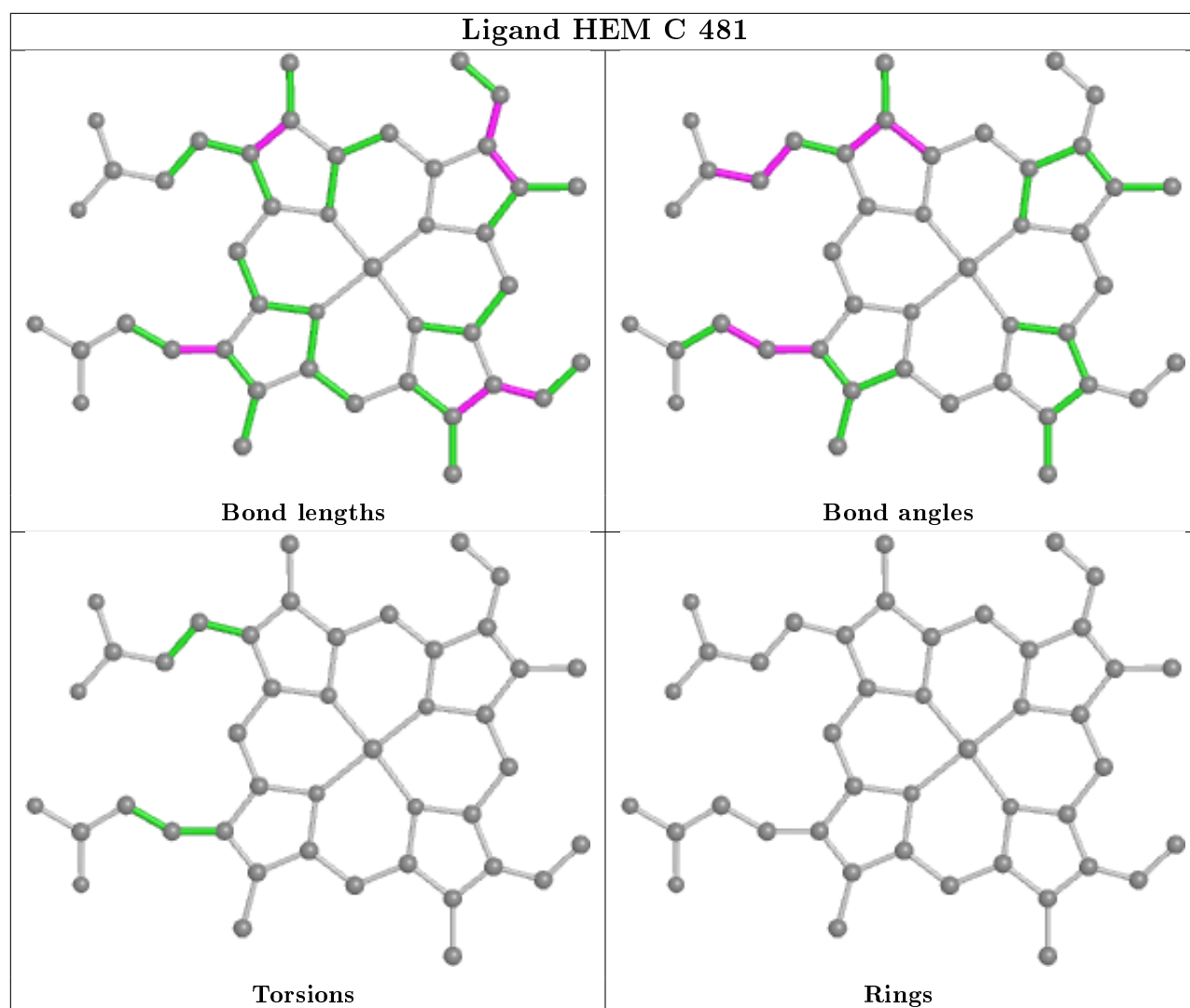


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	448/453 (98%)	0.57	38 (8%) 10 13	37, 55, 77, 97	0
1	B	449/453 (99%)	0.64	41 (9%) 9 10	33, 57, 75, 97	0
1	C	447/453 (98%)	0.81	58 (12%) 3 4	33, 57, 76, 88	0
1	D	445/453 (98%)	0.90	55 (12%) 4 4	22, 54, 75, 98	0
All	All	1789/1812 (98%)	0.73	192 (10%) 6 6	22, 56, 76, 98	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	251	ALA	11.7
1	B	274	ARG	7.7
1	D	257	THR	7.4
1	D	250	GLU	7.2
1	C	29	GLY	6.9
1	D	158	ASN	6.8
1	D	447	LEU	6.7
1	D	256	ASN	6.7
1	D	331	TYR	6.6
1	B	140	ASN	6.2
1	D	248	LYS	6.1
1	C	255	THR	6.1
1	B	257	THR	6.0
1	C	31	LEU	5.9
1	C	139	GLN	5.9
1	B	255	THR	5.8
1	A	255	THR	5.5
1	C	161	GLU	5.4
1	A	254	ASP	5.1
1	B	139	GLN	5.1
1	B	248	LYS	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	274	ARG	5.0
1	A	138	PHE	4.9
1	A	257	THR	4.9
1	D	258	SER	4.9
1	A	139	GLN	4.8
1	D	159	LYS	4.8
1	C	254	ASP	4.7
1	B	244	ILE	4.7
1	D	437	ALA	4.6
1	B	254	ASP	4.5
1	B	249	GLU	4.5
1	D	139	GLN	4.4
1	D	244	ILE	4.4
1	C	366	VAL	4.2
1	C	368	VAL	4.2
1	A	252	GLN	4.1
1	C	252	GLN	4.1
1	A	161	GLU	4.1
1	B	128	PHE	4.0
1	D	136	ALA	4.0
1	D	137	LYS	4.0
1	C	251	ALA	4.0
1	B	50	LYS	3.9
1	B	265	LEU	3.9
1	A	37	GLY	3.8
1	A	38	THR	3.6
1	B	251	ALA	3.6
1	D	66	ILE	3.6
1	C	257	THR	3.6
1	B	253	LYS	3.6
1	C	36	HIS	3.5
1	D	50	LYS	3.5
1	A	472	TYR	3.5
1	C	410	GLY	3.5
1	B	327	ALA	3.5
1	B	320	GLN	3.5
1	C	37	GLY	3.5
1	A	251	ALA	3.5
1	B	250	GLU	3.4
1	A	269	TYR	3.4
1	D	334	VAL	3.4
1	C	38	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	66	ILE	3.3
1	D	187	LEU	3.3
1	C	248	LYS	3.3
1	D	157	TRP	3.3
1	A	440	LEU	3.2
1	B	448	LEU	3.2
1	D	161	GLU	3.2
1	D	446	GLU	3.2
1	A	42	VAL	3.1
1	D	337	GLU	3.1
1	D	160	ASP	3.1
1	B	138	PHE	3.1
1	C	253	LYS	3.1
1	B	266	GLY	3.0
1	A	250	GLU	3.0
1	A	327	ALA	3.0
1	C	327	ALA	3.0
1	A	72	CYS	3.0
1	C	304	LEU	3.0
1	A	273	THR	3.0
1	C	120	PRO	3.0
1	D	476	LYS	3.0
1	D	31	LEU	3.0
1	D	32	PRO	2.9
1	B	258	SER	2.9
1	A	324	GLU	2.9
1	A	128	PHE	2.9
1	C	94	GLU	2.9
1	C	249	GLU	2.9
1	C	448	LEU	2.8
1	D	183	PHE	2.8
1	C	43	GLY	2.8
1	D	29	GLY	2.8
1	B	476	LYS	2.8
1	D	53	LEU	2.8
1	B	119	TYR	2.8
1	A	456	TYR	2.7
1	D	371	TYR	2.7
1	B	318	LEU	2.7
1	A	198	GLN	2.7
1	A	253	LYS	2.7
1	D	57	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	36	HIS	2.7
1	C	206	CYS	2.7
1	A	473	ILE	2.7
1	C	224	GLN	2.6
1	D	365	PRO	2.6
1	D	448	LEU	2.6
1	D	325	PHE	2.6
1	C	457	HIS	2.6
1	A	63	TYR	2.6
1	C	451	LEU	2.6
1	D	407	LEU	2.6
1	C	237	ASP	2.6
1	D	241	GLU	2.6
1	B	242	ILE	2.6
1	A	367	GLN	2.5
1	C	324	GLU	2.5
1	C	65	GLY	2.5
1	B	324	GLU	2.5
1	C	189	LYS	2.5
1	B	252	GLN	2.5
1	D	318	LEU	2.5
1	A	49	GLY	2.5
1	C	55	PHE	2.5
1	C	93	ASN	2.5
1	C	365	PRO	2.5
1	D	473	ILE	2.5
1	C	78	VAL	2.5
1	D	269	TYR	2.5
1	B	247	GLU	2.4
1	B	337	GLU	2.4
1	B	473	ILE	2.4
1	B	256	ASN	2.4
1	C	460	VAL	2.4
1	D	249	GLU	2.4
1	D	408	VAL	2.4
1	C	157	TRP	2.4
1	C	162	GLY	2.4
1	B	273	THR	2.4
1	B	270	ARG	2.4
1	D	396	PRO	2.4
1	C	138	PHE	2.3
1	C	227	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	376	GLY	2.3
1	C	44	HIS	2.3
1	A	248	LYS	2.3
1	B	269	TYR	2.3
1	A	245	ALA	2.3
1	D	150	ARG	2.3
1	D	373	VAL	2.3
1	A	60	LYS	2.3
1	B	460	VAL	2.2
1	C	185	GLU	2.2
1	B	290	ALA	2.2
1	C	226	TYR	2.2
1	A	162	GLY	2.2
1	C	471	LYS	2.2
1	D	322	ILE	2.2
1	C	369	GLY	2.2
1	D	128	PHE	2.2
1	C	33	PRO	2.2
1	A	109	PHE	2.2
1	C	372	VAL	2.2
1	A	476	LYS	2.2
1	B	41	PHE	2.1
1	D	227	ARG	2.1
1	C	476	LYS	2.1
1	A	249	GLU	2.1
1	C	47	GLN	2.1
1	D	445	PHE	2.1
1	A	50	LYS	2.1
1	B	246	ARG	2.1
1	C	473	ILE	2.1
1	C	250	GLU	2.1
1	C	269	TYR	2.1
1	C	274	ARG	2.1
1	D	243	ILE	2.1
1	A	471	LYS	2.1
1	C	439	VAL	2.1
1	B	336	GLU	2.1
1	D	222	LEU	2.0
1	B	345	ALA	2.0
1	D	329	LEU	2.0
1	B	123	ARG	2.0
1	D	119	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	256	ASN	2.0
1	C	64	GLY	2.0
1	D	275	MET	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 carbohydrates in this entry.

6.4 Ligands [i](#)

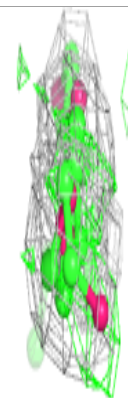
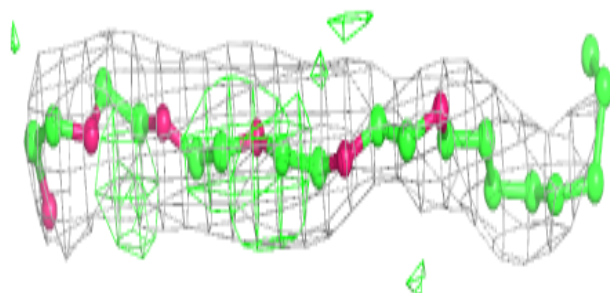
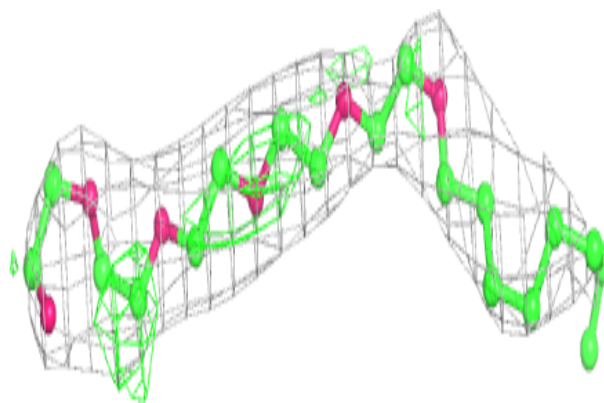
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	N8E	C	1	24/24	0.83	0.42	59,70,75,76	0
2	HEM	A	481	43/43	0.94	0.27	26,51,58,63	0
3	TPF	D	490	22/22	0.94	0.24	53,56,68,69	0
3	TPF	A	490	22/22	0.95	0.21	29,56,73,75	0
3	TPF	B	490	22/22	0.96	0.19	30,62,76,77	0
3	TPF	C	490	22/22	0.96	0.17	32,52,63,66	0
2	HEM	C	481	43/43	0.97	0.25	42,53,68,85	0
2	HEM	B	481	43/43	0.98	0.27	38,56,61,66	0
2	HEM	D	481	43/43	0.99	0.26	51,59,64,64	0

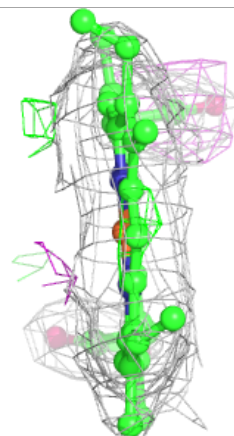
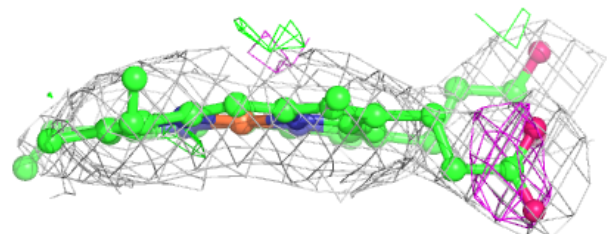
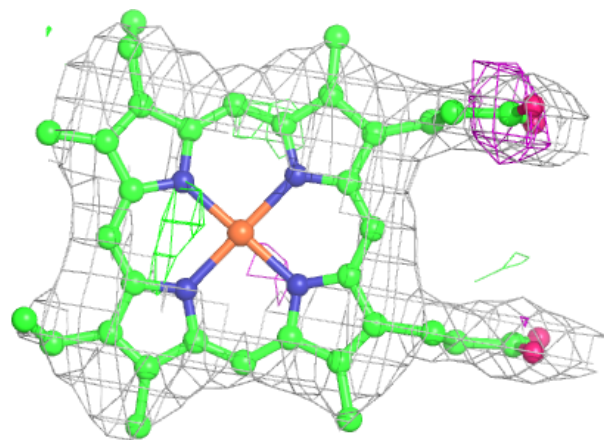
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around N8E C 1:

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

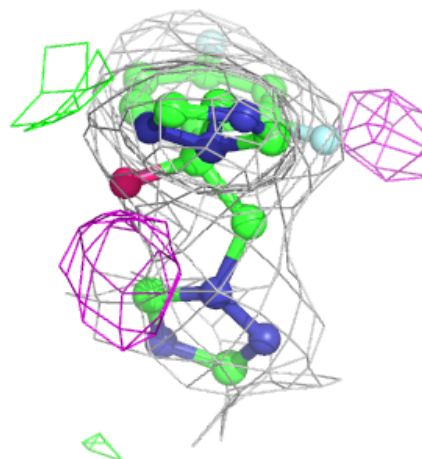
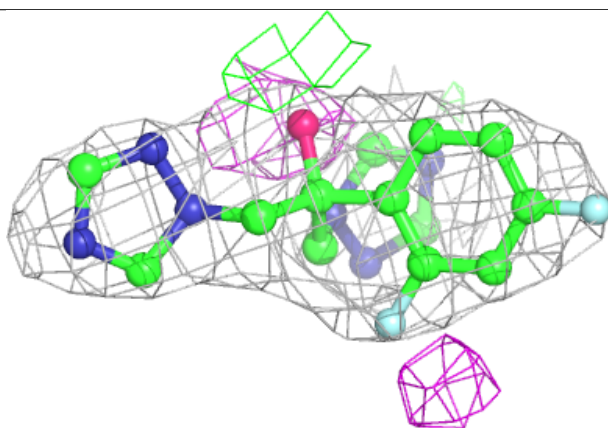
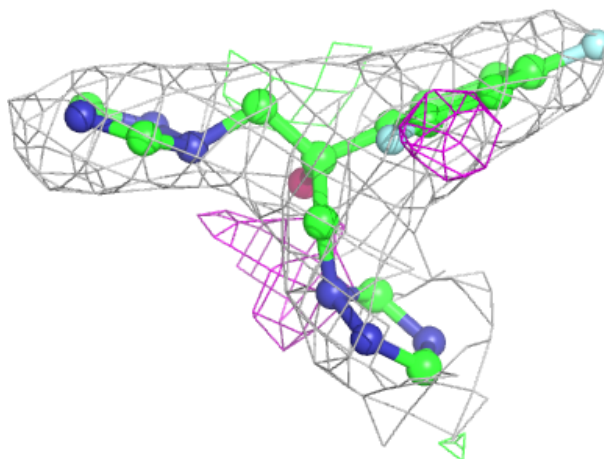
**Electron density around HEM A 481:**

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



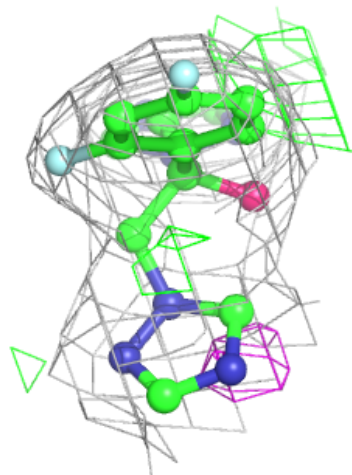
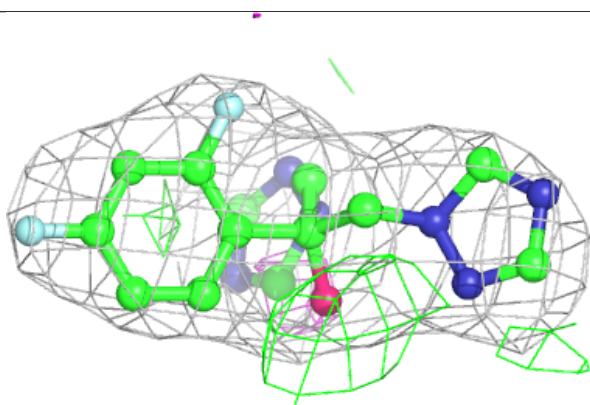
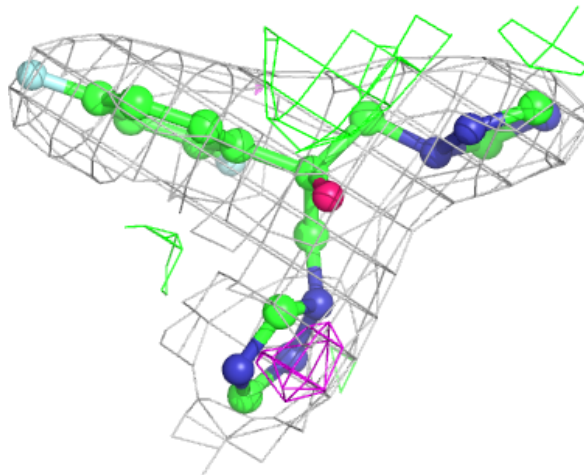
Electron density around TPF D 490:

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



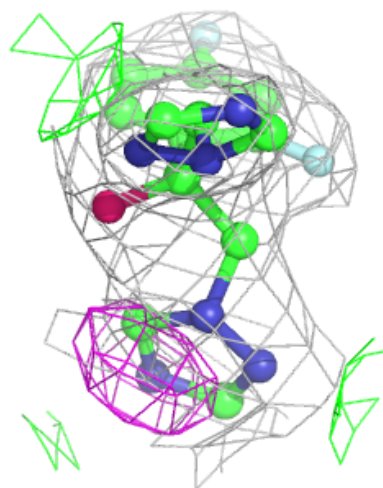
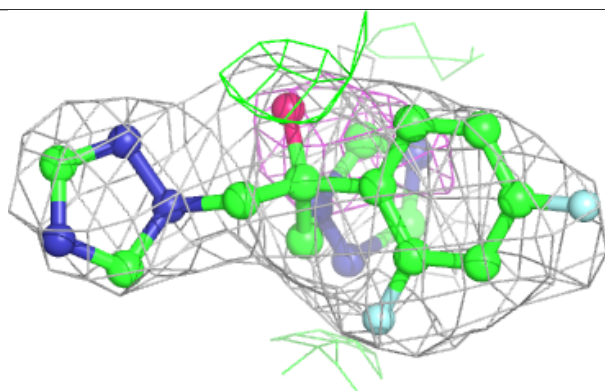
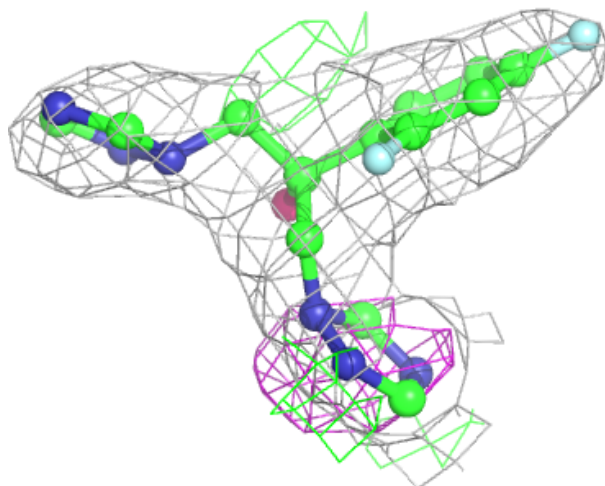
Electron density around TPF A 490:

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



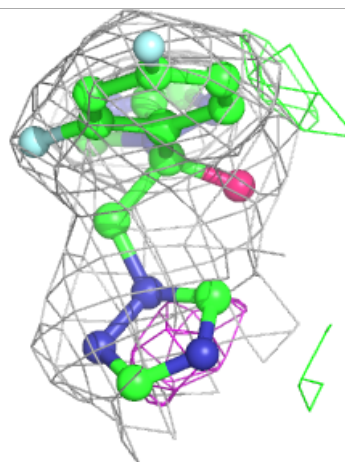
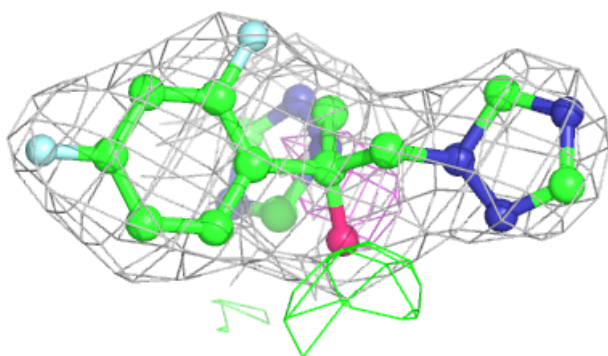
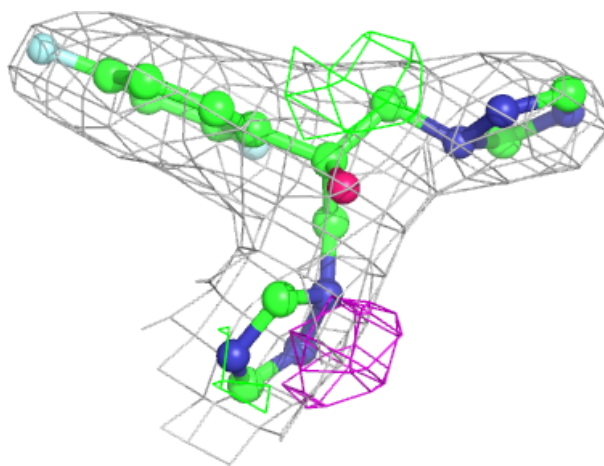
Electron density around TPF B 490:

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



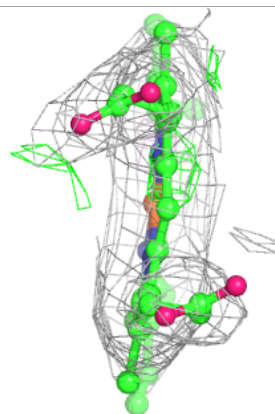
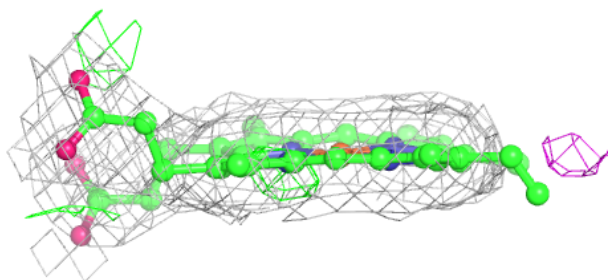
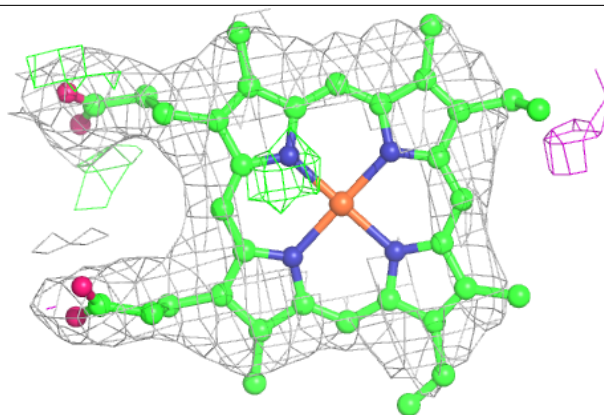
Electron density around TPF C 490:

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



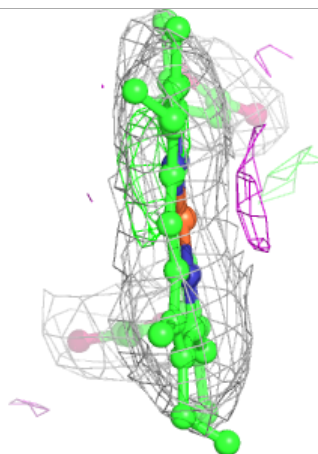
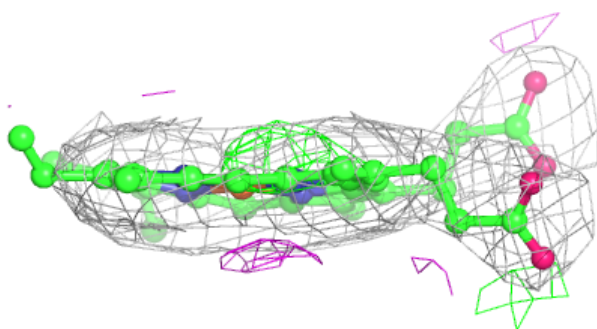
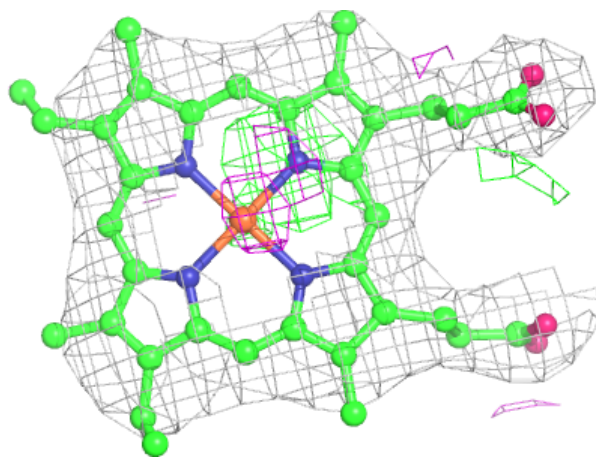
Electron density around HEM C 481:

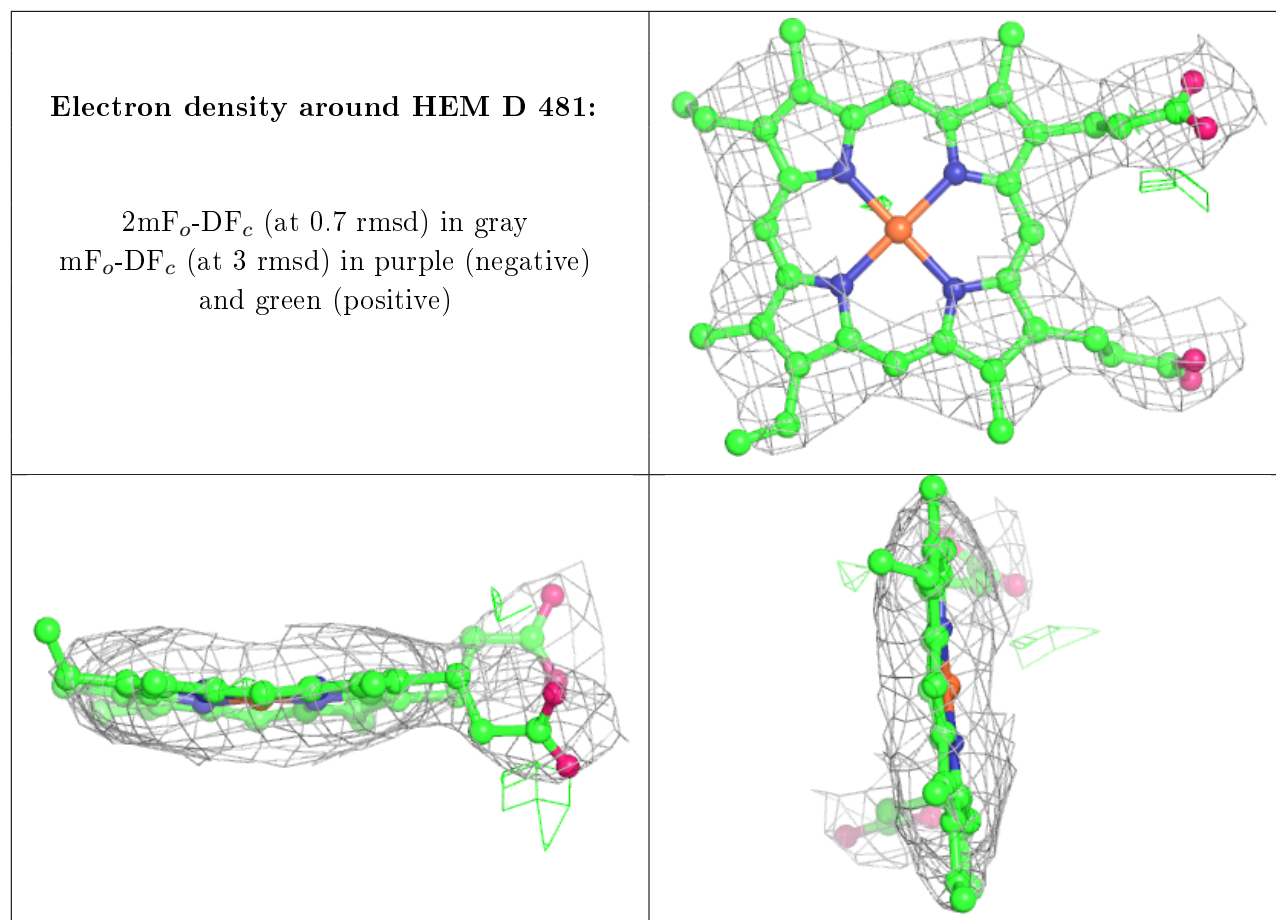
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 481:

$2mF_o-DF_c$ (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.