



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 08:58 AM EDT

PDB ID : 6W32  
Title : Crystal structure of Sfh5  
Authors : Gulten, G.; Khan, D.; Aggarwal, A.; Krieger, I.; Sacchettini, J.C.; Bankaitis, V.A.  
Deposited on : 2020-03-08  
Resolution : 2.90 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
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) : 2.37.1

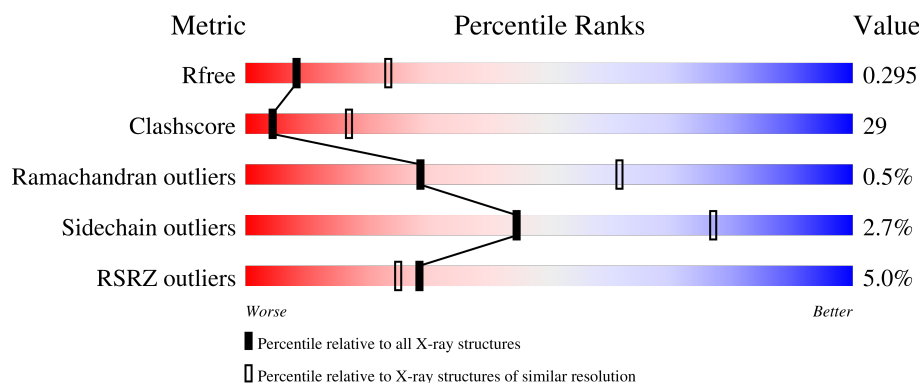
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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	304	
1	B	304	
1	C	304	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7169 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 Phosphatidylinositol transfer protein SFH5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	288	Total	C	N	O	S	0	0	0
			2383	1541	387	446	9			
1	A	278	Total	C	N	O	S	0	0	0
			2296	1488	372	428	8			
1	C	286	Total	C	N	O	S	0	0	0
			2361	1528	383	441	9			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	initiating methionine	UNP A6ZQI5
B	-8	GLY	-	expression tag	UNP A6ZQI5
B	-7	HIS	-	expression tag	UNP A6ZQI5
B	-6	HIS	-	expression tag	UNP A6ZQI5
B	-5	HIS	-	expression tag	UNP A6ZQI5
B	-4	HIS	-	expression tag	UNP A6ZQI5
B	-3	HIS	-	expression tag	UNP A6ZQI5
B	-2	HIS	-	expression tag	UNP A6ZQI5
B	-1	HIS	-	expression tag	UNP A6ZQI5
B	0	HIS	-	expression tag	UNP A6ZQI5
A	-9	MET	-	initiating methionine	UNP A6ZQI5
A	-8	GLY	-	expression tag	UNP A6ZQI5
A	-7	HIS	-	expression tag	UNP A6ZQI5
A	-6	HIS	-	expression tag	UNP A6ZQI5
A	-5	HIS	-	expression tag	UNP A6ZQI5
A	-4	HIS	-	expression tag	UNP A6ZQI5
A	-3	HIS	-	expression tag	UNP A6ZQI5
A	-2	HIS	-	expression tag	UNP A6ZQI5
A	-1	HIS	-	expression tag	UNP A6ZQI5
A	0	HIS	-	expression tag	UNP A6ZQI5
C	-9	MET	-	initiating methionine	UNP A6ZQI5
C	-8	GLY	-	expression tag	UNP A6ZQI5
C	-7	HIS	-	expression tag	UNP A6ZQI5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	HIS	-	expression tag	UNP A6ZQI5
C	-5	HIS	-	expression tag	UNP A6ZQI5
C	-4	HIS	-	expression tag	UNP A6ZQI5
C	-3	HIS	-	expression tag	UNP A6ZQI5
C	-2	HIS	-	expression tag	UNP A6ZQI5
C	-1	HIS	-	expression tag	UNP A6ZQI5
C	0	HIS	-	expression tag	UNP A6ZQI5

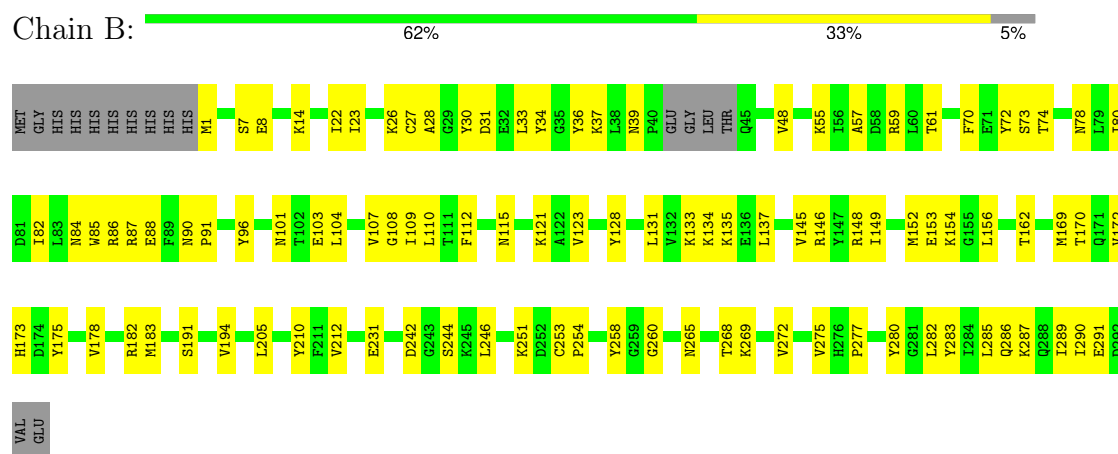
- # HEM

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

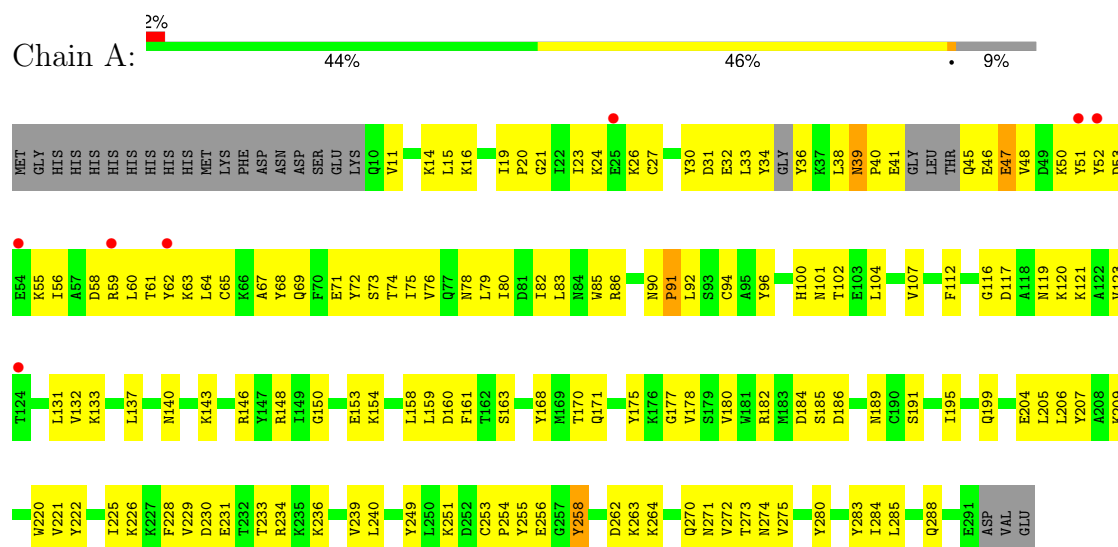
### 3 Residue-property plots

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

#### • Molecule 1: Phosphatidylinositol transfer protein SFH5

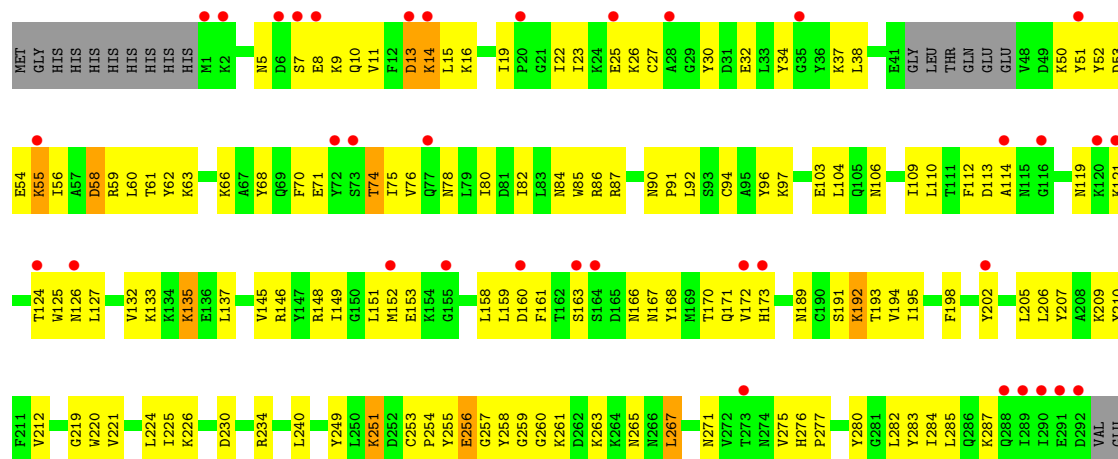


#### • Molecule 1: Phosphatidylinositol transfer protein SFH5



#### • Molecule 1: Phosphatidylinositol transfer protein SFH5





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	205.34Å 205.34Å 68.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.32 – 2.90 29.32 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.32-2.90) 99.5 (29.32-2.90)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.229 , 0.302 0.236 , 0.295	Depositor DCC
$R_{free}$ test set	1649 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.5	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7169	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.60	0/2346	0.72	0/3166
1	B	0.67	0/2435	0.75	0/3282
1	C	0.51	0/2413	0.66	0/3254
All	All	0.60	0/7194	0.71	0/9702

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2296	0	2277	176	0
1	B	2383	0	2373	83	0
1	C	2361	0	2349	152	0
2	A	43	0	30	8	0
2	B	43	0	30	4	0
2	C	43	0	30	2	0
All	All	7169	0	7089	409	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.



All (409) 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:C:253:CYS:O	1:C:260:GLY:HA3	1.35	1.25
1:B:34:TYR:CE1	1:B:205:LEU:HD11	1.74	1.22
1:A:50:LYS:HE3	1:A:51:TYR:CE2	1.77	1.19
1:B:33:LEU:HG	1:B:34:TYR:HD2	1.21	1.00
1:B:33:LEU:HG	1:B:34:TYR:CD2	1.98	0.99
1:C:114:ALA:HA	1:C:121:LYS:HD2	1.40	0.99
1:B:34:TYR:CE1	1:B:205:LEU:CD1	2.53	0.91
1:A:50:LYS:HE3	1:A:51:TYR:HE2	1.14	0.90
1:A:60:LEU:O	1:A:63:LYS:HB3	1.70	0.90
1:A:195:ILE:HD11	2:A:301:HEM:HAD1	1.53	0.90
1:C:255:TYR:HA	1:C:260:GLY:H	1.37	0.89
1:B:34:TYR:HE1	1:B:205:LEU:HD11	1.36	0.88
1:B:34:TYR:HE1	1:B:205:LEU:CD1	1.87	0.86
1:A:23:ILE:HA	1:A:27:CYS:HB2	1.57	0.86
1:A:94:CYS:SG	1:A:146:ARG:NH1	2.48	0.86
1:C:22:ILE:HD11	1:C:23:ILE:CD1	2.07	0.85
1:C:253:CYS:O	1:C:260:GLY:CA	2.23	0.85
1:A:69:GLN:O	1:A:71:GLU:HG3	1.78	0.83
1:C:16:LYS:HA	1:C:19:ILE:HG23	1.61	0.83
1:B:107:VAL:HG21	1:B:131:LEU:HD11	1.61	0.81
1:C:5:ASN:HD22	1:C:8:GLU:HG3	1.43	0.81
1:C:58:ASP:O	1:C:61:THR:HG22	1.80	0.81
1:C:255:TYR:HB2	1:C:260:GLY:O	1.80	0.81
1:C:255:TYR:CA	1:C:260:GLY:H	1.94	0.81
1:A:170:THR:HG22	1:A:207:TYR:HB3	1.62	0.80
1:A:50:LYS:CE	1:A:51:TYR:HE2	1.92	0.80
1:C:74:THR:HG22	1:C:78:ASN:HD22	1.47	0.79
1:C:22:ILE:HD11	1:C:23:ILE:HD12	1.64	0.79
1:A:41:GLU:O	1:A:48:VAL:HG21	1.83	0.79
1:C:11:VAL:HG11	1:C:70:PHE:HD1	1.48	0.79
1:C:23:ILE:HA	1:C:27:CYS:HB2	1.64	0.78
1:A:34:TYR:HA	1:A:86:ARG:NH2	1.98	0.78
1:A:63:LYS:HD2	1:A:204:GLU:O	1.83	0.77
1:A:34:TYR:HA	1:A:86:ARG:HH22	1.50	0.77
1:A:79:LEU:O	1:A:79:LEU:HD23	1.85	0.76
1:C:168:TYR:HB3	1:C:207:TYR:HB2	1.67	0.75
1:C:92:LEU:H	1:C:92:LEU:HD23	1.52	0.74
1:A:55:LYS:O	1:A:59:ARG:HG3	1.88	0.74
1:B:55:LYS:O	1:B:59:ARG:HG2	1.86	0.74
1:A:20:PRO:O	1:A:24:LYS:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ARG:O	1:A:62:TYR:HB3	1.88	0.72
1:C:19:ILE:HA	1:C:22:ILE:HG12	1.72	0.72
1:A:34:TYR:CE1	1:A:205:LEU:HD11	2.24	0.72
1:C:94:CYS:SG	1:C:146:ARG:NH1	2.62	0.72
1:A:50:LYS:CE	1:A:51:TYR:CE2	2.67	0.71
1:A:38:LEU:HA	1:A:52:TYR:HE1	1.56	0.70
1:A:32:GLU:OE2	1:A:92:LEU:HD11	1.91	0.70
1:C:16:LYS:HE2	1:C:38:LEU:HD23	1.71	0.70
1:A:60:LEU:O	1:A:64:LEU:N	2.25	0.70
1:A:33:LEU:HD23	1:A:60:LEU:HD12	1.72	0.69
1:C:109:ILE:HD12	1:C:267:LEU:CD2	2.23	0.69
1:A:60:LEU:HD21	1:A:161:PHE:CD1	2.28	0.69
1:C:22:ILE:CD1	1:C:23:ILE:CD1	2.70	0.68
1:C:86:ARG:HE	1:C:91:PRO:HG2	1.58	0.68
1:C:60:LEU:HD22	1:C:161:PHE:CD2	2.28	0.68
1:B:145:VAL:O	1:B:149:ILE:HG12	1.94	0.67
1:A:60:LEU:O	1:A:63:LYS:CB	2.40	0.67
1:C:37:LYS:HD3	1:C:52:TYR:HD1	1.58	0.67
1:C:172:VAL:HG22	1:C:210:TYR:HB2	1.77	0.67
1:C:22:ILE:HD11	1:C:23:ILE:HD11	1.77	0.66
1:A:60:LEU:O	1:A:63:LYS:N	2.28	0.66
1:C:22:ILE:HG13	1:C:23:ILE:HG13	1.77	0.66
1:C:63:LYS:O	1:C:66:LYS:N	2.29	0.66
1:B:55:LYS:NZ	1:B:162:THR:HG21	2.09	0.66
1:C:60:LEU:CD2	1:C:161:PHE:HB3	2.26	0.66
1:A:171:GLN:HB2	1:A:209:LYS:HD2	1.78	0.66
1:A:74:THR:O	1:A:78:ASN:ND2	2.28	0.66
1:B:268:THR:HG21	1:A:102:THR:HG22	1.78	0.65
1:A:90:ASN:N	1:A:91:PRO:HD3	2.12	0.65
1:C:255:TYR:O	1:C:256:GLU:HB3	1.96	0.65
1:A:107:VAL:HG21	1:A:131:LEU:HD21	1.79	0.64
1:C:11:VAL:HG11	1:C:70:PHE:CD1	2.31	0.64
1:C:58:ASP:OD2	1:C:58:ASP:N	2.28	0.64
1:C:10:GLN:O	1:C:14:LYS:HE3	1.96	0.64
1:C:126:ASN:OD1	1:C:148:ARG:NH1	2.29	0.64
1:B:86:ARG:NH1	1:B:153:GLU:OE2	2.29	0.64
1:B:265:ASN:HB2	1:B:269:LYS:HB2	1.80	0.64
1:B:31:ASP:OD2	1:B:39:ASN:HB3	1.98	0.64
1:B:101:ASN:OD1	1:B:103:GLU:HG2	1.98	0.64
1:A:33:LEU:HB2	1:A:38:LEU:HD11	1.80	0.64
1:C:170:THR:HG22	1:C:207:TYR:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LEU:CD2	1:A:161:PHE:CD1	2.81	0.63
1:C:74:THR:HG22	1:C:78:ASN:ND2	2.14	0.63
1:A:280:TYR:O	1:A:284:ILE:HD12	1.99	0.63
1:A:86:ARG:NH1	1:A:153:GLU:OE2	2.32	0.63
1:C:189:ASN:O	1:C:193:THR:HG23	1.98	0.62
1:B:154:LYS:HD3	1:B:275:VAL:HG11	1.81	0.62
1:C:30:TYR:CE2	1:C:32:GLU:HB3	2.34	0.62
1:C:255:TYR:HA	1:C:260:GLY:N	2.12	0.62
1:A:274:ASN:O	1:A:274:ASN:ND2	2.33	0.62
1:A:60:LEU:O	1:A:63:LYS:CA	2.48	0.62
1:A:20:PRO:HD2	1:A:21:GLY:H	1.63	0.62
1:A:132:VAL:HG21	1:A:178:VAL:HA	1.81	0.62
1:A:180:VAL:HG11	1:C:219:GLY:HA3	1.80	0.62
1:C:68:TYR:HB2	1:C:75:ILE:HG12	1.82	0.61
1:C:103:GLU:HA	1:C:106:ASN:ND2	2.14	0.61
1:A:33:LEU:HD22	1:A:38:LEU:HD11	1.83	0.61
1:A:45:GLN:HG3	1:A:45:GLN:O	1.99	0.61
1:A:73:SER:HA	1:A:76:VAL:HG12	1.82	0.61
1:C:109:ILE:HD12	1:C:267:LEU:HD23	1.82	0.61
1:B:55:LYS:HE2	1:B:162:THR:CG2	2.30	0.61
1:A:180:VAL:CG1	1:C:219:GLY:HA3	2.31	0.61
1:A:39:ASN:HD22	1:A:40:PRO:HD2	1.66	0.61
1:A:195:ILE:CD1	2:A:301:HEM:HAD1	2.29	0.61
1:A:199:GLN:OE1	1:A:233:THR:HG21	2.01	0.61
1:A:284:ILE:HD12	1:A:284:ILE:H	1.67	0.60
1:A:38:LEU:CA	1:A:52:TYR:HE1	2.15	0.60
1:C:78:ASN:O	1:C:82:ILE:HG13	2.02	0.60
1:C:22:ILE:CD1	1:C:23:ILE:HD12	2.30	0.60
1:C:60:LEU:CD2	1:C:161:PHE:CD2	2.84	0.60
1:B:110:LEU:O	1:B:272:VAL:HG23	2.02	0.59
1:B:283:TYR:CE2	1:B:287:LYS:HE3	2.37	0.59
1:A:86:ARG:HD2	1:A:91:PRO:HG2	1.85	0.59
1:A:33:LEU:O	1:A:34:TYR:C	2.39	0.59
1:C:74:THR:O	1:C:75:ILE:C	2.41	0.59
1:C:104:LEU:HG	1:C:137:LEU:HD23	1.83	0.59
1:C:282:LEU:HD12	1:C:285:LEU:HB2	1.84	0.59
1:A:19:ILE:HG12	1:A:20:PRO:HD3	1.85	0.59
1:A:38:LEU:HA	1:A:52:TYR:CE1	2.37	0.59
1:B:57:ALA:O	1:B:61:THR:HG23	2.03	0.59
1:A:16:LYS:NZ	1:A:16:LYS:HB3	2.17	0.59
1:C:22:ILE:HG13	1:C:23:ILE:CG1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:VAL:HG12	1:C:240:LEU:HB2	1.85	0.59
1:A:76:VAL:O	1:A:80:ILE:HG23	2.03	0.58
1:C:60:LEU:HD21	1:C:161:PHE:CB	2.32	0.58
1:C:254:PRO:O	1:C:255:TYR:HB3	2.02	0.58
1:C:8:GLU:O	1:C:11:VAL:HG22	2.04	0.58
1:C:280:TYR:CE2	1:C:284:ILE:HD11	2.38	0.58
1:B:183:MET:SD	2:B:301:HEM:HBB2	2.44	0.58
1:B:282:LEU:O	1:B:286:GLN:HG2	2.04	0.58
1:C:37:LYS:HD3	1:C:52:TYR:CD1	2.38	0.58
1:C:226:LYS:O	1:C:234:ARG:NH1	2.37	0.57
1:C:27:CYS:HA	1:C:84:ASN:HD21	1.69	0.57
1:A:225:ILE:O	1:A:228:PHE:N	2.33	0.57
1:A:47:GLU:HA	1:A:51:TYR:CD2	2.40	0.57
1:A:50:LYS:HB2	1:A:51:TYR:CD2	2.40	0.57
1:A:30:TYR:CE2	1:A:32:GLU:CB	2.87	0.57
1:B:242:ASP:OD1	1:B:244:SER:OG	2.22	0.57
1:C:113:ASP:O	1:C:121:LYS:HG2	2.05	0.57
1:C:255:TYR:CD2	1:C:256:GLU:N	2.73	0.57
1:C:282:LEU:HA	1:C:285:LEU:HD12	1.85	0.57
1:A:233:THR:HA	1:A:236:LYS:HE3	1.87	0.57
1:B:96:TYR:CE2	1:B:277:PRO:HB3	2.40	0.56
1:B:175:TYR:O	1:B:178:VAL:HG22	2.05	0.56
1:B:133:LYS:HB2	1:B:134:LYS:HG2	1.86	0.56
1:A:14:LYS:HB2	1:A:72:TYR:CD1	2.41	0.56
1:A:46:GLU:OE1	1:A:46:GLU:HA	2.05	0.56
1:C:59:ARG:O	1:C:62:TYR:HB3	2.05	0.56
1:C:60:LEU:HD22	1:C:161:PHE:HD2	1.68	0.56
1:C:34:TYR:CZ	1:C:205:LEU:HD11	2.41	0.56
1:C:125:TRP:CZ3	1:C:258:TYR:CE1	2.93	0.56
1:C:53:ASP:OD1	1:C:55:LYS:N	2.38	0.56
1:C:253:CYS:SG	1:C:260:GLY:CA	2.93	0.56
1:A:65:CYS:SG	1:A:75:ILE:HD13	2.46	0.56
1:A:90:ASN:HD21	1:A:288:GLN:HE22	1.53	0.56
1:C:22:ILE:HG13	1:C:23:ILE:N	2.21	0.55
1:C:51:TYR:HD2	1:C:283:TYR:HD2	1.52	0.55
1:B:152:MET:SD	1:B:169:MET:HE1	2.46	0.55
1:A:60:LEU:HD21	1:A:161:PHE:CE1	2.41	0.55
1:C:7:SER:HA	1:C:10:GLN:HB2	1.88	0.55
1:C:253:CYS:C	1:C:260:GLY:HA3	2.22	0.55
1:A:39:ASN:HD21	1:A:41:GLU:HG3	1.72	0.55
1:A:53:ASP:O	1:A:55:LYS:N	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:LYS:HG3	1:C:285:LEU:HD22	1.88	0.55
1:A:116:GLY:N	1:A:121:LYS:HE2	2.22	0.55
1:C:112:PHE:HE2	1:C:158:LEU:O	1.89	0.55
1:A:30:TYR:CE2	1:A:32:GLU:HB3	2.42	0.55
1:C:71:GLU:O	1:C:75:ILE:HG13	2.06	0.55
1:B:1:MET:HB3	1:B:59:ARG:NH2	2.22	0.54
1:C:109:ILE:HD12	1:C:267:LEU:HD21	1.88	0.54
1:C:283:TYR:O	1:C:287:LYS:HB2	2.07	0.54
1:A:90:ASN:O	1:A:92:LEU:N	2.40	0.54
1:A:16:LYS:HA	1:A:19:ILE:HG23	1.88	0.54
1:A:199:GLN:HE22	1:A:230:ASP:H	1.54	0.54
1:A:39:ASN:ND2	1:A:40:PRO:HD2	2.21	0.54
1:A:47:GLU:CA	1:A:51:TYR:HD2	2.21	0.54
1:C:124:THR:HB	1:C:151:LEU:HD21	1.89	0.54
1:C:210:TYR:HH	1:C:249:TYR:HD1	1.54	0.54
1:A:19:ILE:CD1	1:A:40:PRO:HG3	2.38	0.54
1:A:33:LEU:CD2	1:A:60:LEU:CD1	2.86	0.54
1:C:34:TYR:H	1:C:86:ARG:HH22	1.55	0.54
1:B:27:CYS:SG	1:B:80:ILE:HD13	2.48	0.54
1:A:38:LEU:C	1:A:52:TYR:HE1	2.10	0.54
1:B:37:LYS:HE3	1:B:39:ASN:O	2.07	0.54
1:B:283:TYR:HE2	1:B:287:LYS:HE3	1.72	0.54
1:B:14:LYS:HD3	1:B:72:TYR:CE1	2.42	0.54
1:A:119:ASN:O	1:A:170:THR:HG23	2.08	0.54
1:C:90:ASN:N	1:C:146:ARG:HH22	2.06	0.54
1:A:33:LEU:HD23	1:A:60:LEU:CD1	2.38	0.53
1:C:189:ASN:HA	1:C:192:LYS:HG3	1.89	0.53
1:B:34:TYR:HD1	1:B:156:LEU:HD13	1.74	0.53
1:A:30:TYR:CE2	1:A:32:GLU:HB2	2.44	0.53
1:A:120:LYS:NZ	1:A:249:TYR:O	2.24	0.53
1:A:82:ILE:O	1:A:86:ARG:HG2	2.08	0.53
1:C:112:PHE:HD2	1:C:158:LEU:HD23	1.74	0.53
1:A:14:LYS:HE3	1:A:72:TYR:HD1	1.74	0.53
1:A:231:GLU:HG2	1:A:234:ARG:NH2	2.23	0.53
1:C:160:ASP:HB2	1:C:166:ASN:HB3	1.91	0.53
1:A:14:LYS:HB2	1:A:72:TYR:CE1	2.44	0.52
1:C:11:VAL:O	1:C:15:LEU:HB2	2.09	0.52
1:C:97:LYS:HE2	1:C:285:LEU:HD22	1.91	0.52
1:B:34:TYR:CZ	1:B:205:LEU:HD11	2.36	0.52
1:A:15:LEU:O	1:A:19:ILE:N	2.43	0.52
1:A:47:GLU:HA	1:A:51:TYR:HD2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:LEU:HD23	1:B:137:LEU:HD13	1.92	0.51
1:C:225:ILE:HG21	2:C:301:HEM:C2D	2.46	0.51
1:C:251:LYS:O	1:C:261:LYS:HG3	2.10	0.51
1:A:222:TYR:CE2	1:A:226:LYS:HD3	2.45	0.51
1:A:31:ASP:HB3	1:A:39:ASN:HB2	1.92	0.51
1:A:254:PRO:HD3	1:A:270:GLN:OE1	2.11	0.51
1:C:22:ILE:CD1	1:C:23:ILE:HD11	2.38	0.51
1:A:60:LEU:HA	1:A:63:LYS:HB3	1.92	0.51
1:A:60:LEU:CD2	1:A:161:PHE:CE1	2.94	0.51
1:A:67:ALA:HB2	1:A:204:GLU:CG	2.41	0.51
1:A:132:VAL:HG11	1:A:177:GLY:O	2.10	0.51
1:C:52:TYR:CE2	1:C:54:GLU:HG3	2.46	0.51
1:A:140:ASN:ND2	1:A:143:LYS:HB2	2.26	0.51
1:A:175:TYR:CE1	2:A:301:HEM:C4B	2.98	0.51
1:A:15:LEU:HD11	1:A:75:ILE:HG21	1.92	0.51
1:A:26:LYS:O	1:A:26:LYS:HD3	2.10	0.51
1:A:123:VAL:HA	1:A:170:THR:O	2.10	0.51
1:C:13:ASP:N	1:C:13:ASP:OD1	2.42	0.51
1:B:74:THR:O	1:B:78:ASN:ND2	2.39	0.50
1:A:39:ASN:HD22	1:A:40:PRO:CD	2.23	0.50
1:C:22:ILE:CG1	1:C:23:ILE:HD12	2.41	0.50
1:A:31:ASP:HB2	1:A:39:ASN:H	1.76	0.50
1:C:114:ALA:CA	1:C:121:LYS:HD2	2.29	0.50
1:C:119:ASN:O	1:C:170:THR:HG23	2.10	0.50
1:A:117:ASP:OD2	1:A:251:LYS:NZ	2.45	0.50
1:C:125:TRP:HZ3	1:C:258:TYR:CE1	2.30	0.50
1:A:19:ILE:O	1:A:23:ILE:HG13	2.11	0.50
1:A:191:SER:HB2	2:A:301:HEM:C2A	2.47	0.50
1:B:96:TYR:CD2	1:B:277:PRO:HB3	2.47	0.50
1:C:171:GLN:HE21	1:C:206:LEU:HG	1.76	0.50
1:C:198:PHE:HA	1:C:202:TYR:HB2	1.94	0.50
1:A:33:LEU:CD2	1:A:60:LEU:HD13	2.42	0.49
1:A:220:TRP:CE2	1:A:221:VAL:HG23	2.47	0.49
1:A:186:ASP:O	1:A:189:ASN:N	2.46	0.49
1:B:30:TYR:CD1	1:B:87:ARG:HG2	2.48	0.49
1:B:254:PRO:HG2	1:B:258:TYR:HD2	1.75	0.49
1:C:255:TYR:CD1	1:C:259:GLY:HA2	2.47	0.49
1:A:60:LEU:HA	1:A:63:LYS:CB	2.42	0.49
1:A:199:GLN:NE2	1:A:230:ASP:H	2.10	0.49
1:A:90:ASN:N	1:A:91:PRO:CD	2.75	0.49
1:B:55:LYS:CE	1:B:162:THR:HG21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:ILE:CA	1:C:22:ILE:HG12	2.43	0.49
1:A:79:LEU:HD23	1:A:79:LEU:C	2.31	0.48
1:C:96:TYR:CE1	1:C:277:PRO:HB3	2.48	0.48
1:C:132:VAL:HG13	1:C:133:LYS:H	1.79	0.48
1:B:104:LEU:HG	1:B:137:LEU:HD22	1.95	0.48
1:C:60:LEU:O	1:C:63:LYS:N	2.44	0.48
1:A:58:ASP:O	1:A:61:THR:HB	2.12	0.48
1:B:30:TYR:HB2	1:B:87:ARG:HD3	1.94	0.48
1:C:159:LEU:HB2	1:C:161:PHE:CE1	2.48	0.48
1:C:253:CYS:SG	1:C:260:GLY:HA2	2.54	0.48
1:C:210:TYR:OH	1:C:249:TYR:HB3	2.14	0.48
1:C:275:VAL:HG23	1:C:276:HIS:H	1.79	0.48
1:A:39:ASN:ND2	1:A:41:GLU:HG3	2.29	0.48
1:A:33:LEU:CD2	1:A:38:LEU:HD11	2.43	0.47
1:A:33:LEU:CB	1:A:38:LEU:HD11	2.43	0.47
1:A:112:PHE:HB2	1:A:158:LEU:HD23	1.95	0.47
1:C:159:LEU:HA	1:C:166:ASN:OD1	2.14	0.47
1:A:14:LYS:HE3	1:A:72:TYR:CD1	2.49	0.47
1:A:60:LEU:CA	1:A:63:LYS:HB3	2.45	0.47
1:B:286:GLN:O	1:B:289:ILE:HG12	2.15	0.47
1:A:233:THR:O	1:A:236:LYS:HG3	2.13	0.47
1:A:209:LYS:HE2	2:A:301:HEM:HBD1	1.96	0.47
1:C:60:LEU:HD21	1:C:161:PHE:CG	2.50	0.47
1:C:167:ASN:OD1	1:C:167:ASN:N	2.41	0.47
1:A:19:ILE:HD11	1:A:40:PRO:HG3	1.95	0.47
1:A:231:GLU:HG2	1:A:234:ARG:CZ	2.45	0.47
1:C:14:LYS:HD2	1:C:15:LEU:N	2.29	0.47
1:C:90:ASN:H	1:C:146:ARG:HH22	1.62	0.47
1:B:85:TRP:CZ3	1:B:91:PRO:HG3	2.50	0.47
1:A:100:HIS:O	1:A:143:LYS:NZ	2.42	0.47
1:C:173:HIS:NE2	2:C:301:HEM:O2A	2.46	0.47
1:A:56:ILE:O	1:A:59:ARG:N	2.47	0.47
1:A:133:LYS:HE3	1:A:182:ARG:NH1	2.29	0.47
1:A:60:LEU:C	1:A:63:LYS:HB3	2.33	0.47
1:A:100:HIS:C	1:A:143:LYS:HZ1	2.18	0.47
1:B:90:ASN:H	1:B:146:ARG:HH12	1.62	0.46
1:C:85:TRP:CZ3	1:C:202:TYR:HE1	2.33	0.46
1:B:107:VAL:HG11	1:B:131:LEU:HD11	1.97	0.46
1:B:128:TYR:OH	1:B:148:ARG:HD3	2.16	0.46
1:C:149:ILE:O	1:C:152:MET:HB3	2.14	0.46
1:C:8:GLU:O	1:C:11:VAL:CG2	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ALA:O	1:B:30:TYR:N	2.49	0.46
1:A:30:TYR:HE2	1:A:32:GLU:HB3	1.80	0.46
1:A:255:TYR:HB3	1:A:263:LYS:HA	1.97	0.46
1:A:15:LEU:O	1:A:19:ILE:HG23	2.16	0.46
1:A:150:GLY:O	1:A:154:LYS:HG3	2.15	0.46
1:A:160:ASP:O	1:A:163:SER:HB3	2.16	0.46
1:A:271:ASN:OD1	1:A:272:VAL:N	2.44	0.46
1:C:255:TYR:CA	1:C:260:GLY:N	2.70	0.46
1:C:74:THR:CG2	1:C:78:ASN:ND2	2.78	0.46
1:C:92:LEU:H	1:C:92:LEU:CD2	2.26	0.46
1:A:191:SER:HB2	2:A:301:HEM:C1A	2.51	0.46
1:B:172:VAL:HG22	1:B:210:TYR:HB2	1.98	0.46
1:A:63:LYS:CD	1:A:204:GLU:O	2.61	0.46
1:B:37:LYS:HE2	1:B:48:VAL:HG12	1.98	0.46
1:A:229:VAL:HB	1:A:233:THR:OG1	2.16	0.46
1:A:16:LYS:HE2	1:A:58:ASP:CG	2.36	0.46
1:A:19:ILE:CG1	1:A:20:PRO:HD3	2.46	0.46
1:A:34:TYR:CA	1:A:86:ARG:NH2	2.74	0.46
1:B:34:TYR:O	1:B:36:TYR:CD2	2.70	0.45
1:C:265:ASN:OD1	1:C:265:ASN:N	2.49	0.45
1:A:68:TYR:CE1	1:A:78:ASN:CG	2.90	0.45
1:B:23:ILE:O	1:B:27:CYS:HB2	2.17	0.45
1:B:37:LYS:HG3	1:B:280:TYR:CZ	2.50	0.45
1:A:263:LYS:HB3	1:A:263:LYS:HE3	1.72	0.45
2:A:301:HEM:CHA	2:A:301:HEM:HBA2	2.45	0.45
1:C:34:TYR:H	1:C:86:ARG:NH2	2.13	0.45
1:B:55:LYS:HZ1	1:B:162:THR:HG21	1.81	0.45
1:C:255:TYR:HB2	1:C:260:GLY:N	2.32	0.45
1:B:135:LYS:HE3	1:B:182:ARG:HB3	1.99	0.45
1:B:253:CYS:O	1:B:260:GLY:HA3	2.16	0.45
1:A:222:TYR:O	1:A:226:LYS:HG3	2.16	0.45
1:B:84:ASN:O	1:B:88:GLU:HG3	2.17	0.45
1:C:30:TYR:CD1	1:C:87:ARG:HG2	2.51	0.45
1:C:275:VAL:HG23	1:C:276:HIS:N	2.31	0.45
1:A:184:ASP:OD1	1:A:185:SER:N	2.50	0.45
1:C:76:VAL:O	1:C:80:ILE:HG13	2.17	0.45
1:C:263:LYS:HB3	1:C:263:LYS:HE2	1.74	0.45
1:A:19:ILE:HG13	1:A:40:PRO:HG3	1.99	0.44
1:B:104:LEU:HA	1:B:104:LEU:HD23	1.75	0.44
1:B:55:LYS:HE2	1:B:162:THR:HG21	1.98	0.44
1:B:103:GLU:OE1	1:A:273:THR:OG1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ILE:HD12	1:B:291:GLU:N	2.33	0.44
1:B:55:LYS:CE	1:B:162:THR:HB	2.47	0.44
1:B:123:VAL:HA	1:B:170:THR:O	2.17	0.44
1:A:262:ASP:C	1:A:264:LYS:H	2.19	0.44
1:B:26:LYS:HB2	1:B:80:ILE:HD12	1.99	0.44
1:A:85:TRP:O	1:A:86:ARG:C	2.55	0.44
1:A:64:LEU:HG	1:A:64:LEU:O	2.18	0.44
1:A:96:TYR:HE1	1:A:275:VAL:HG23	1.83	0.44
1:A:53:ASP:C	1:A:55:LYS:H	2.19	0.43
1:C:91:PRO:HD2	1:C:92:LEU:HD23	1.99	0.43
1:C:125:TRP:CD2	1:C:267:LEU:HD11	2.53	0.43
1:A:15:LEU:HD11	1:A:75:ILE:CG2	2.48	0.43
1:A:20:PRO:CD	1:A:21:GLY:H	2.30	0.43
1:C:224:LEU:HD12	1:C:224:LEU:O	2.18	0.43
1:A:132:VAL:CG2	1:A:178:VAL:HA	2.47	0.43
1:A:153:GLU:HA	1:A:153:GLU:OE1	2.19	0.43
1:C:50:LYS:O	1:C:52:TYR:N	2.50	0.43
1:C:60:LEU:CD2	1:C:161:PHE:CB	2.93	0.43
1:C:160:ASP:HB2	1:C:166:ASN:CB	2.48	0.43
1:C:19:ILE:HG22	1:C:22:ILE:HD13	2.01	0.43
1:C:25:GLU:HB3	1:C:26:LYS:HE2	1.99	0.43
1:C:74:THR:O	1:C:76:VAL:N	2.52	0.43
1:C:60:LEU:HD23	1:C:161:PHE:HB3	2.00	0.43
1:C:112:PHE:CD2	1:C:158:LEU:HD23	2.54	0.43
1:C:191:SER:O	1:C:195:ILE:HG13	2.18	0.43
1:C:103:GLU:HA	1:C:106:ASN:HD22	1.79	0.43
1:A:38:LEU:C	1:A:52:TYR:CE1	2.92	0.43
1:C:91:PRO:HB2	1:C:153:GLU:OE2	2.19	0.43
1:B:112:PHE:HA	1:B:121:LYS:O	2.19	0.43
1:B:285:LEU:HD23	1:B:285:LEU:HA	1.72	0.43
1:C:145:VAL:HG23	1:C:194:VAL:HG22	2.01	0.43
1:A:47:GLU:CA	1:A:51:TYR:CD2	2.99	0.42
1:A:230:ASP:N	1:A:230:ASP:OD1	2.52	0.42
1:B:8:GLU:HG2	1:B:70:PHE:CG	2.54	0.42
1:A:206:LEU:HD11	1:A:209:LYS:HB2	2.01	0.42
1:C:135:LYS:HD2	1:C:135:LYS:O	2.19	0.42
1:C:206:LEU:HD23	1:C:207:TYR:N	2.35	0.42
1:A:39:ASN:HD22	1:A:39:ASN:C	2.23	0.42
1:C:56:ILE:HD12	1:C:161:PHE:O	2.19	0.42
1:C:86:ARG:NE	1:C:91:PRO:HG2	2.30	0.42
1:B:194:VAL:CG1	2:B:301:HEM:HBA1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:VAL:HG11	1:B:246:LEU:HD13	2.02	0.42
1:A:104:LEU:HD23	1:A:104:LEU:HA	1.94	0.42
1:B:1:MET:HB3	1:B:59:ARG:HH22	1.85	0.42
1:B:231:GLU:OE2	1:B:231:GLU:N	2.53	0.42
1:C:220:TRP:CE2	1:C:221:VAL:HG23	2.55	0.42
1:B:172:VAL:HG21	1:B:246:LEU:HD21	2.01	0.42
2:A:301:HEM:HBA2	2:A:301:HEM:HHA	2.02	0.42
1:A:285:LEU:HD23	1:A:285:LEU:HA	1.85	0.41
1:A:258:TYR:CD2	1:A:258:TYR:N	2.87	0.41
1:C:37:LYS:CD	1:C:52:TYR:HD1	2.30	0.41
1:B:251:LYS:HB3	1:B:251:LYS:HE2	1.78	0.41
1:A:39:ASN:HD22	1:A:40:PRO:N	2.18	0.41
1:C:110:LEU:O	1:C:271:ASN:HA	2.20	0.41
1:B:169:MET:HE3	1:B:169:MET:HB3	1.75	0.41
1:A:119:ASN:HB3	1:A:168:TYR:HB2	2.02	0.41
1:A:239:VAL:O	1:A:240:LEU:HD23	2.20	0.41
1:A:16:LYS:HB3	1:A:16:LYS:HZ2	1.85	0.41
1:A:137:LEU:HD23	1:A:137:LEU:HA	1.85	0.41
1:C:74:THR:CG2	1:C:78:ASN:HD22	2.26	0.41
1:C:171:GLN:HB2	1:C:209:LYS:HD2	2.03	0.41
1:B:22:ILE:HG23	1:B:80:ILE:HD11	2.03	0.41
1:B:55:LYS:HE2	1:B:162:THR:HB	2.03	0.41
1:A:256:GLU:O	1:A:256:GLU:HG2	2.21	0.41
1:B:33:LEU:CG	1:B:34:TYR:CD2	2.87	0.41
1:B:135:LYS:NZ	1:B:182:ARG:O	2.54	0.41
1:A:11:VAL:O	1:A:11:VAL:HG23	2.21	0.41
1:A:33:LEU:O	1:A:36:TYR:N	2.54	0.41
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.88	0.41
1:C:255:TYR:HB2	1:C:260:GLY:C	2.41	0.41
1:B:82:ILE:O	1:B:86:ARG:HG2	2.22	0.40
1:B:173:HIS:ND1	1:B:175:TYR:OH	2.40	0.40
1:A:27:CYS:SG	1:A:83:LEU:HD12	2.61	0.40
1:A:225:ILE:O	1:A:226:LYS:C	2.58	0.40
1:A:280:TYR:O	1:A:283:TYR:HB3	2.21	0.40
1:C:113:ASP:O	1:C:121:LYS:CG	2.68	0.40
1:B:175:TYR:CE1	2:B:301:HEM:C4B	3.09	0.40
1:B:194:VAL:HG11	2:B:301:HEM:HBA1	2.02	0.40
1:A:101:ASN:HB2	1:A:143:LYS:HZ1	1.86	0.40
1:C:254:PRO:O	1:C:255:TYR:CB	2.69	0.40
1:B:108:GLY:O	1:B:109:ILE:HD13	2.21	0.40
1:A:21:GLY:HA2	1:A:24:LYS:CB	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	272/304 (90%)	229 (84%)	42 (15%)	1 (0%)	34	66
1	B	284/304 (93%)	263 (93%)	21 (7%)	0	100	100
1	C	282/304 (93%)	232 (82%)	47 (17%)	3 (1%)	14	42
All	All	838/912 (92%)	724 (86%)	110 (13%)	4 (0%)	29	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	PRO
1	C	163	SER
1	C	55	LYS
1	C	257	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	251/276 (91%)	246 (98%)	5 (2%)	55	82
1	B	262/276 (95%)	258 (98%)	4 (2%)	65	87
1	C	259/276 (94%)	247 (95%)	12 (5%)	27	60
All	All	772/828 (93%)	751 (97%)	21 (3%)	44	77

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	SER
1	B	73	SER
1	B	115	ASN
1	B	191	SER
1	A	39	ASN
1	A	47	GLU
1	A	148	ARG
1	A	253	CYS
1	A	258	TYR
1	C	9	LYS
1	C	13	ASP
1	C	14	LYS
1	C	58	ASP
1	C	74	THR
1	C	127	LEU
1	C	135	LYS
1	C	192	LYS
1	C	230	ASP
1	C	251	LYS
1	C	256	GLU
1	C	267	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	119	ASN
1	A	288	GLN
1	C	5	ASN
1	C	78	ASN
1	C	106	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 monosaccharides in this entry.

## 5.6 Ligand geometry

3 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	C	301	1	42,50,50	1.86	7 (16%)	46,82,82	1.79	8 (17%)
2	HEM	B	301	1	42,50,50	1.94	6 (14%)	46,82,82	2.00	14 (30%)
2	HEM	A	301	1	42,50,50	1.87	7 (16%)	46,82,82	1.91	10 (21%)

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	C	301	1	-	4/12/54/54	-
2	HEM	B	301	1	-	5/12/54/54	-
2	HEM	A	301	1	-	6/12/54/54	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	HEM	C3D-C2D	7.78	1.53	1.36
2	C	301	HEM	C3D-C2D	7.51	1.53	1.36
2	A	301	HEM	C3D-C2D	7.11	1.52	1.36
2	C	301	HEM	C3C-C2C	-4.38	1.34	1.40
2	A	301	HEM	C3C-C2C	-3.97	1.35	1.40
2	A	301	HEM	C3C-C4C	3.89	1.47	1.41
2	B	301	HEM	C3C-CAC	3.62	1.55	1.47
2	B	301	HEM	C3C-C2C	-3.46	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	HEM	C3C-C4C	3.15	1.46	1.41
2	A	301	HEM	CAB-C3B	3.01	1.55	1.47
2	B	301	HEM	CAB-C3B	2.79	1.54	1.47
2	B	301	HEM	C2C-C1C	2.69	1.48	1.42
2	A	301	HEM	C3C-CAC	2.60	1.53	1.47
2	C	301	HEM	C3C-C4C	2.58	1.45	1.41
2	C	301	HEM	C3C-CAC	2.37	1.52	1.47
2	C	301	HEM	CAB-C3B	2.28	1.53	1.47
2	A	301	HEM	CMB-C2B	2.23	1.55	1.50
2	C	301	HEM	O1A-CGA	2.14	1.29	1.22
2	A	301	HEM	CAA-C2A	2.11	1.57	1.52
2	C	301	HEM	CMD-C2D	2.10	1.55	1.50

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	HEM	C4C-CHD-C1D	6.39	131.00	122.56
2	C	301	HEM	C4D-ND-C1D	5.57	111.80	105.21
2	A	301	HEM	C4D-ND-C1D	5.34	111.54	105.21
2	C	301	HEM	C4C-CHD-C1D	5.29	129.54	122.56
2	B	301	HEM	C4B-CHC-C1C	4.42	128.39	122.56
2	B	301	HEM	C4D-ND-C1D	4.09	110.05	105.21
2	B	301	HEM	CMA-C3A-C4A	-4.08	122.47	128.46
2	A	301	HEM	CBA-CAA-C2A	-3.86	106.04	112.54
2	B	301	HEM	C4C-CHD-C1D	3.85	127.64	122.56
2	B	301	HEM	CBA-CAA-C2A	3.55	118.51	112.54
2	B	301	HEM	CMA-C3A-C2A	3.24	131.05	124.94
2	B	301	HEM	C3B-C4B-NB	-3.18	107.19	109.47
2	B	301	HEM	O1A-CGA-CBA	-3.18	113.01	123.09
2	C	301	HEM	CHC-C4B-NB	3.13	127.81	124.44
2	A	301	HEM	C4B-CHC-C1C	3.11	126.66	122.56
2	C	301	HEM	CMA-C3A-C4A	-3.07	123.96	128.46
2	A	301	HEM	CHC-C4B-NB	2.97	127.63	124.44
2	C	301	HEM	C4B-CHC-C1C	2.86	126.33	122.56
2	C	301	HEM	CBB-CAB-C3B	-2.59	114.58	127.53
2	B	301	HEM	CMD-C2D-C1D	2.58	129.07	125.03
2	C	301	HEM	C3C-C4C-NC	-2.54	106.15	110.94
2	B	301	HEM	C3C-C4C-NC	-2.49	106.25	110.94
2	B	301	HEM	C1B-NB-C4B	2.44	108.10	105.21
2	A	301	HEM	C2C-C3C-C4C	2.41	108.58	106.90
2	C	301	HEM	C2C-C3C-C4C	2.39	108.56	106.90
2	A	301	HEM	O1D-CGD-CBD	-2.31	115.77	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	HEM	C3C-C4C-NC	-2.30	106.60	110.94
2	A	301	HEM	CMA-C3A-C4A	-2.18	125.26	128.46
2	B	301	HEM	CHA-C4D-ND	2.16	127.04	124.37
2	B	301	HEM	CBD-CAD-C3D	-2.13	106.64	112.53
2	A	301	HEM	CAD-C3D-C4D	2.12	128.39	124.70
2	B	301	HEM	CAD-CBD-CGD	-2.02	108.30	113.67

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	HEM	C2A-CAA-CBA-CGA
2	A	301	HEM	C2B-C3B-CAB-CBB
2	A	301	HEM	C3A-C2A-CAA-CBA
2	B	301	HEM	C2B-C3B-CAB-CBB
2	A	301	HEM	C1A-C2A-CAA-CBA
2	B	301	HEM	C4B-C3B-CAB-CBB
2	A	301	HEM	C4B-C3B-CAB-CBB
2	B	301	HEM	CAA-CBA-CGA-O1A
2	C	301	HEM	C4B-C3B-CAB-CBB
2	C	301	HEM	CAD-CBD-CGD-O1D
2	A	301	HEM	CAA-CBA-CGA-O1A
2	A	301	HEM	CAD-CBD-CGD-O2D
2	C	301	HEM	C2B-C3B-CAB-CBB
2	C	301	HEM	CAD-CBD-CGD-O2D
2	B	301	HEM	CAD-CBD-CGD-O2D

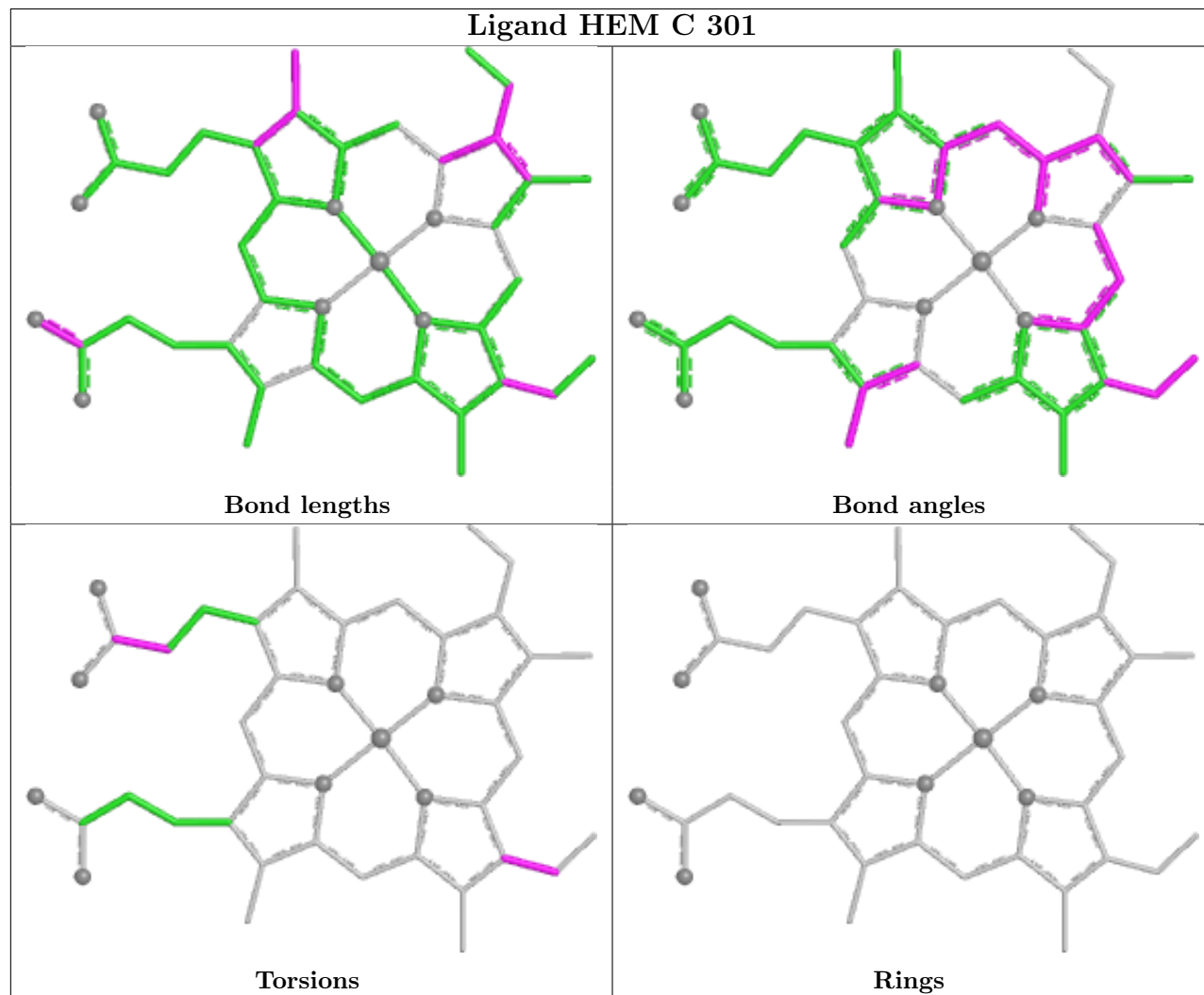
There are no ring outliers.

3 monomers are involved in 14 short contacts:

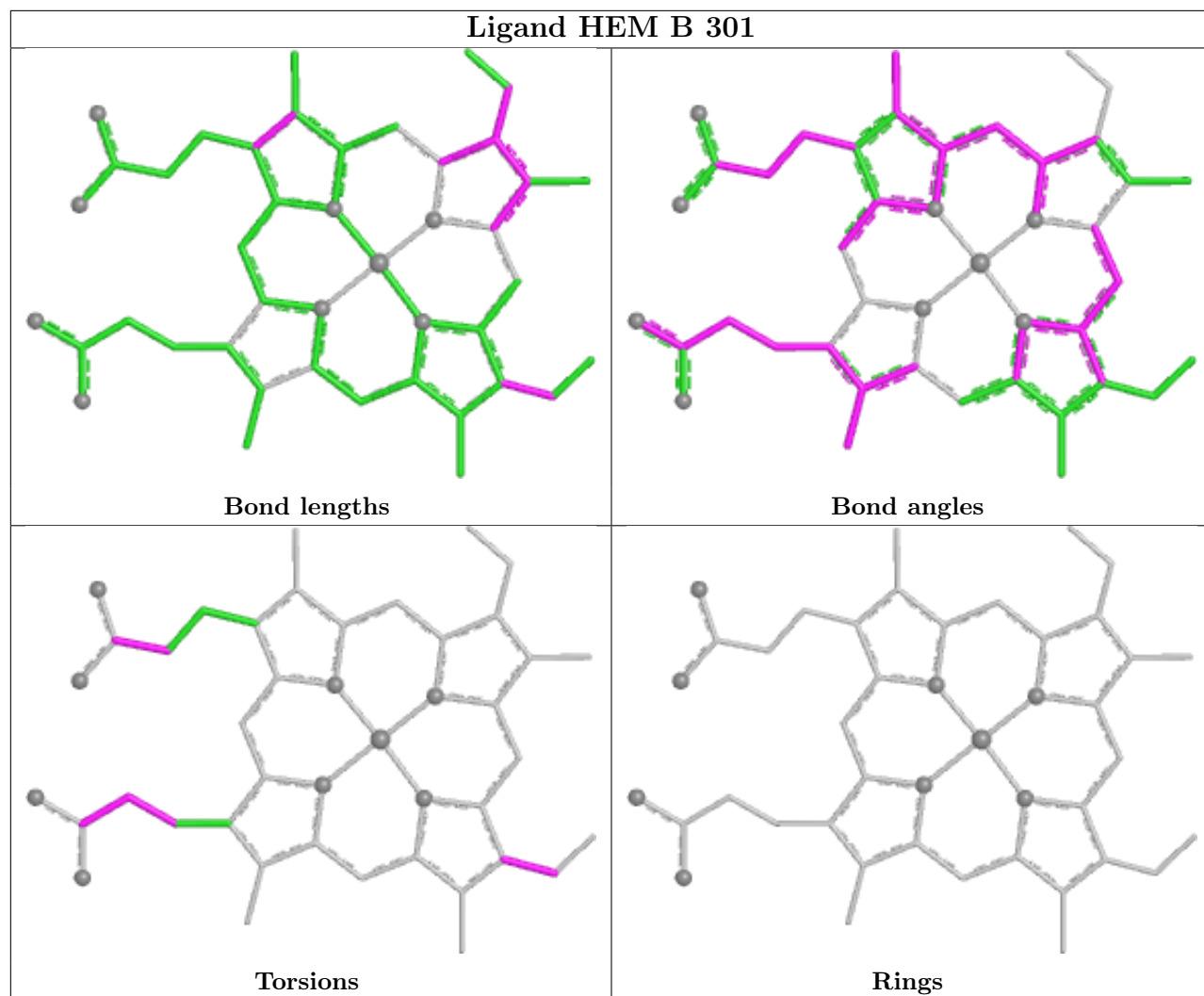
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	HEM	2	0
2	B	301	HEM	4	0
2	A	301	HEM	8	0

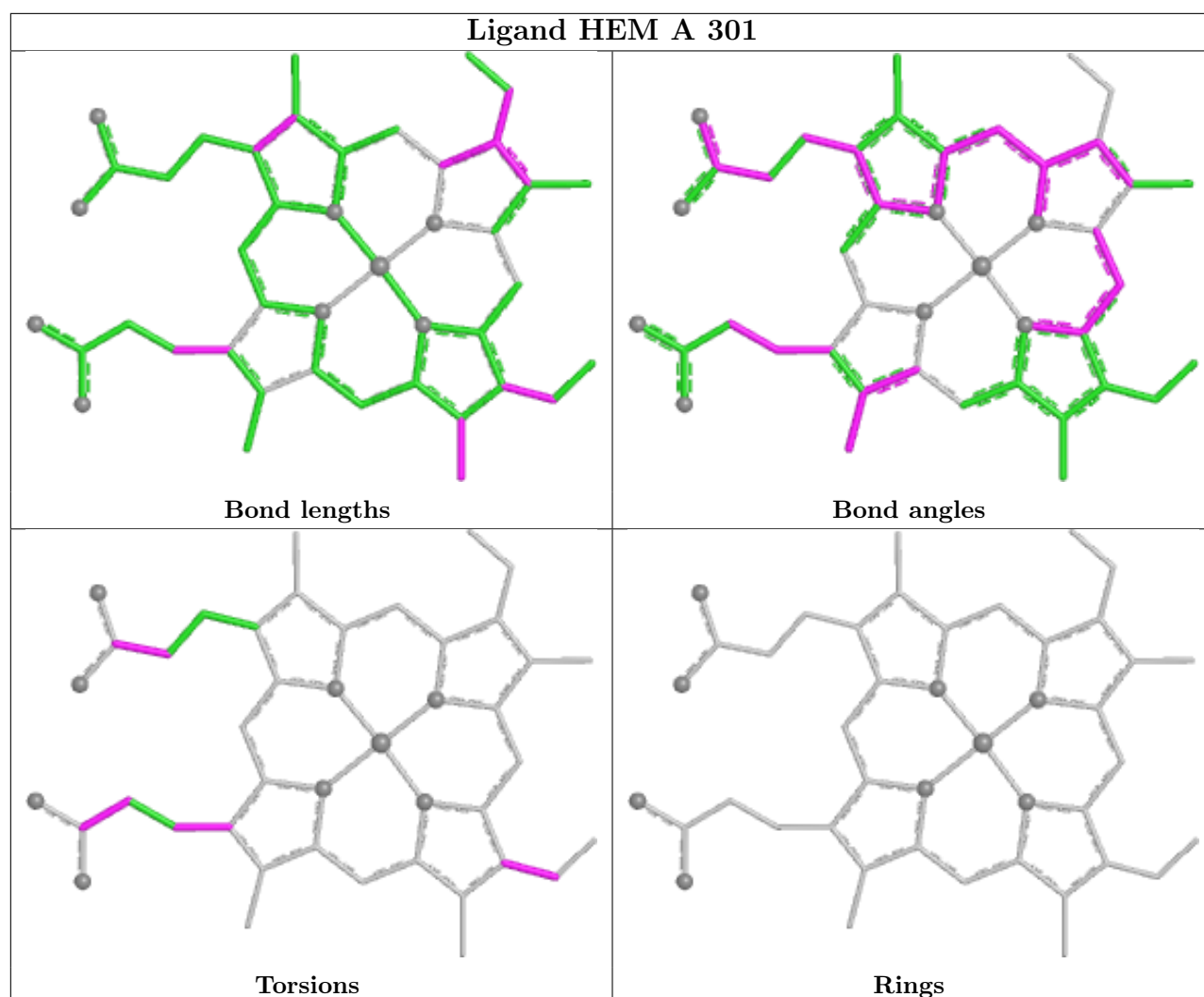
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	278/304 (91%)	0.24	7 (2%) 57 55	55, 82, 109, 119	0
1	B	288/304 (94%)	-0.20	0 100 100	41, 56, 88, 120	1 (0%)
1	C	286/304 (94%)	0.63	36 (12%) 3 3	49, 100, 140, 150	0
All	All	852/912 (93%)	0.22	43 (5%) 28 25	41, 78, 130, 150	1 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	5.9
1	C	7	SER	5.7
1	C	292	ASP	5.6
1	C	290	ILE	5.5
1	C	8	GLU	5.0
1	C	51	TYR	4.1
1	C	72	TYR	4.1
1	C	291	GLU	4.1
1	A	25	GLU	4.0
1	C	73	SER	3.9
1	C	77	GLN	3.8
1	C	121	LYS	3.8
1	A	62	TYR	3.7
1	C	6	ASP	3.4
1	C	288	GLN	3.3
1	C	163	SER	3.2
1	C	13	ASP	3.2
1	C	173	HIS	3.1
1	A	51	TYR	3.1
1	C	289	ILE	3.1
1	A	59	ARG	3.0
1	C	20	PRO	2.8
1	C	164	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	124	THR	2.7
1	C	273	THR	2.6
1	C	126	ASN	2.6
1	C	14	LYS	2.6
1	C	202	TYR	2.5
1	C	2	LYS	2.5
1	A	52	TYR	2.5
1	C	25	GLU	2.5
1	C	35	GLY	2.4
1	C	172	VAL	2.4
1	A	54	GLU	2.2
1	C	55	LYS	2.2
1	C	120	LYS	2.2
1	C	152	MET	2.1
1	C	116	GLY	2.1
1	A	124	THR	2.1
1	C	160	ASP	2.1
1	C	114	ALA	2.1
1	C	155	GLY	2.1
1	C	28	ALA	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](#)

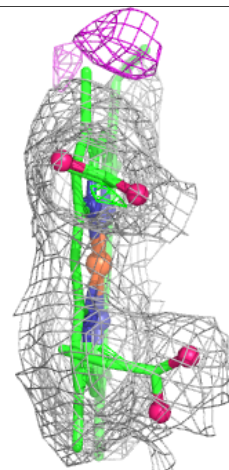
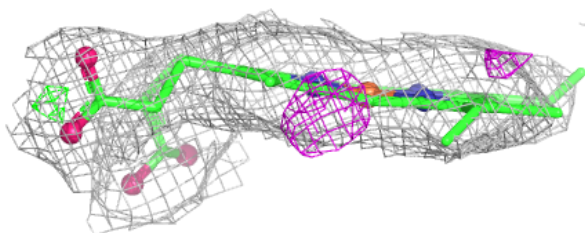
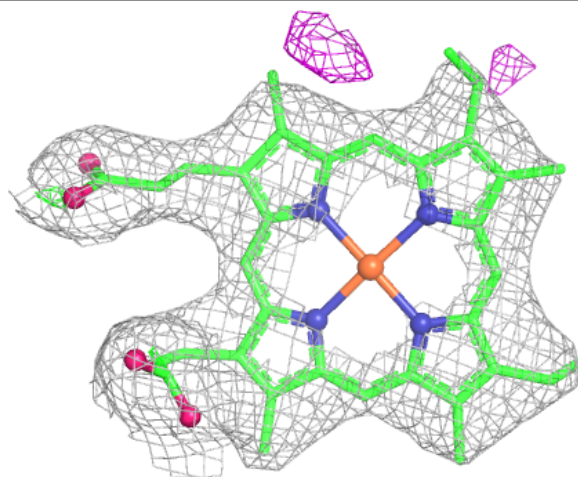
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	HEM	B	301	43/43	0.96	0.24	30,47,54,61	0
2	HEM	C	301	43/43	0.96	0.25	53,62,76,80	0
2	HEM	A	301	43/43	0.97	0.25	55,62,69,72	0

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

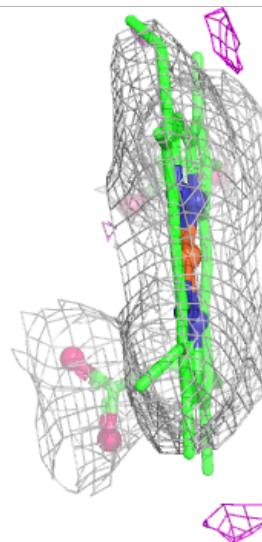
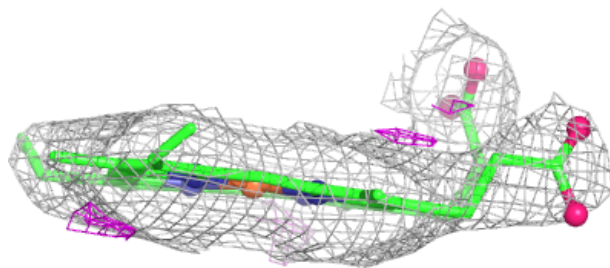
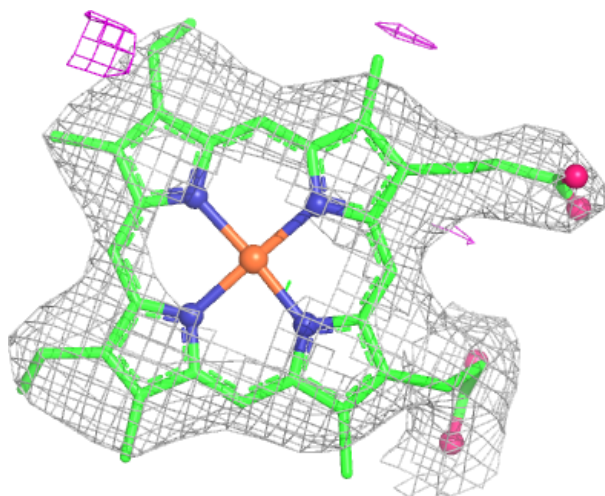
**Electron density around HEM B 301:**

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



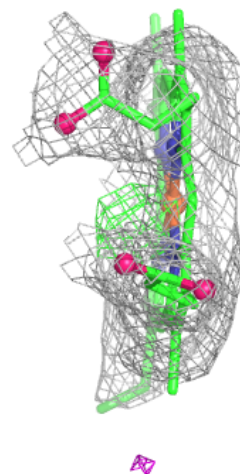
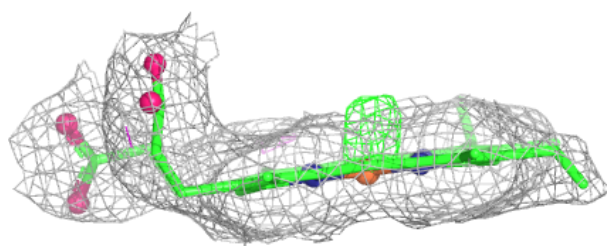
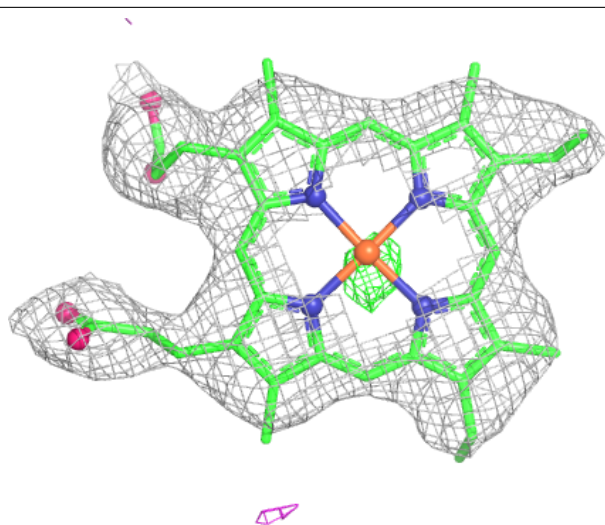
**Electron density around HEM C 301:**

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



**Electron density around HEM A 301:**

$2mF_o-DF_c$  (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.