



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:17 pm BST

PDB ID : 3NW2  
Title : Novel nanomolar Imidazopyridines as selective Nitric Oxide Synthase (iNOS) inhibitors: SAR and structural insights  
Authors : Graedler, U.; Fuchss, T.; Ulrich, W.R.; Boer, R.; Strub, A.; Hesslinger, C.; Anezo, C.; Diederichs, K.; Zaliani, A.  
Deposited on : 2010-07-09  
Resolution : 2.80 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.

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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	:	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

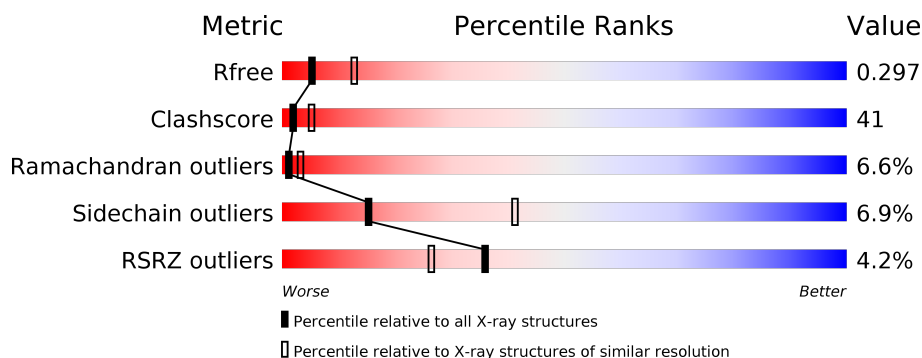
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	423	<div> <div>5%</div> <div> <div></div> <div>40%</div> <div>49%</div> <div>8%</div> <div>••</div> </div> </div>
1	B	423	<div> <div>3%</div> <div> <div></div> <div>39%</div> <div>50%</div> <div>9%</div> <div>•</div> </div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6991 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 Nitric oxide synthase, inducible.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3376	2163	582	611	20			
1	B	413	Total	C	N	O	S	0	0	0
			3368	2159	581	608	20			

- 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	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula:  $C_9H_{15}N_5O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

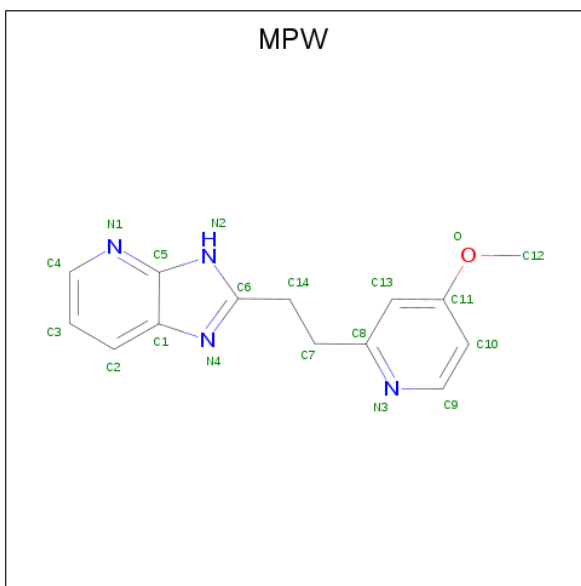
- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 2-[2-(4-methoxypyridin-2-yl)ethyl]-3H-imidazo[4,5-b]pyridine (three-letter

code: MPW) (formula: C<sub>14</sub>H<sub>14</sub>N<sub>4</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			19	14	4	1		
5	B	1	Total	C	N	O	0	0
			19	14	4	1		

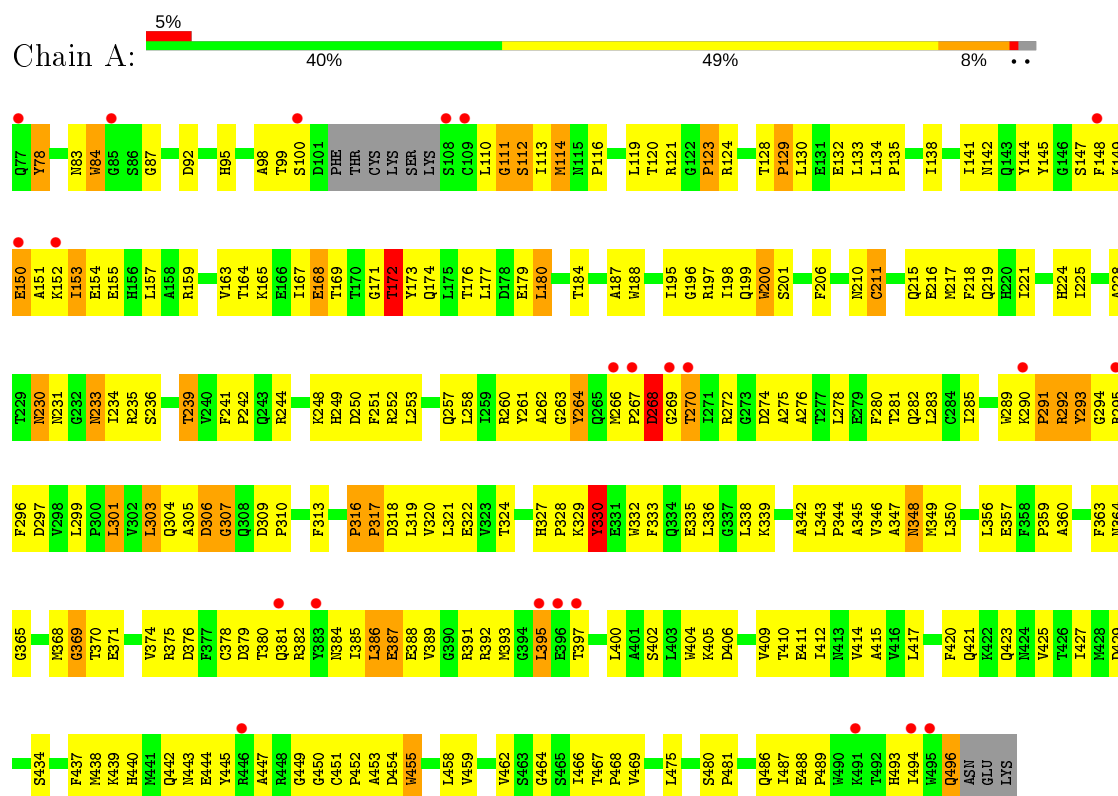
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	40	Total	O	0	0
			40	40		
6	B	44	Total	O	0	0
			44	44		

### 3 Residue-property plots

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: Nitric oxide synthase, inducible





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.60 Å   212.60 Å   111.50 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	19.72 – 2.80 19.72 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.72-2.80) 99.8 (19.72-2.80)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 2.79 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.279   ,   0.323 0.251   ,   0.297	Depositor DCC
$R_{free}$ test set	1824 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.0	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 87.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6991	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, SO4, H4B, MPW

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	0.44	0/3474	0.70	0/4723
1	B	0.43	0/3466	0.70	1/4712 (0.0%)
All	All	0.43	0/6940	0.70	1/9435 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	365	GLY	N-CA-C	-5.15	100.23	113.10

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	3376	0	3269	282	0
1	B	3368	0	3265	276	0
2	A	43	0	30	6	0
2	B	43	0	30	3	0
3	A	17	0	15	1	0
3	B	17	0	15	0	0
4	A	5	0	0	0	0
5	A	19	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	19	0	14	3	0
6	A	40	0	0	9	0
6	B	44	0	0	5	0
All	All	6991	0	6652	560	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 41.

All (560) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:MET:HE3	1:B:469:VAL:HG12	1.25	1.15
1:A:132:GLU:O	1:A:135:PRO:HD2	1.62	0.99
1:A:176:THR:OG1	1:A:179:GLU:HG3	1.61	0.99
1:A:144:TYR:CE1	1:A:179:GLU:HG2	2.00	0.96
1:B:343:LEU:HD11	1:B:364:ASN:HD22	1.31	0.95
1:B:141:ILE:HD13	1:B:163:VAL:HG21	1.49	0.95
1:B:163:VAL:HG12	1:B:167:ILE:HD11	1.49	0.94
1:A:141:ILE:CD1	1:A:163:VAL:HG21	1.97	0.93
1:A:241:PHE:HB3	1:A:242:PRO:CD	2.01	0.90
1:B:141:ILE:CD1	1:B:163:VAL:HG21	2.04	0.88
1:A:138:ILE:HG22	1:A:142:ASN:HD21	1.39	0.88
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.04	0.87
1:B:228:ALA:HB1	1:B:364:ASN:HD21	1.38	0.87
1:A:262:ALA:HB2	1:A:299:LEU:CD2	2.03	0.86
1:A:134:LEU:O	1:A:138:ILE:HG12	1.76	0.86
1:A:195:ILE:HD12	1:A:368:MET:CE	2.07	0.85
1:B:177:LEU:HD13	1:B:181:ILE:HD13	1.58	0.85
1:B:175:LEU:HD23	1:B:356:LEU:HD12	1.58	0.85
1:A:393:MET:HB2	1:A:395:LEU:HD22	1.59	0.85
1:A:330:TYR:HB3	1:A:332:TRP:NE1	1.92	0.84
1:B:159:ARG:O	1:B:163:VAL:HG23	1.76	0.83
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.14	0.83
1:A:141:ILE:HD13	1:A:163:VAL:HG21	1.58	0.83
1:B:176:THR:OG1	1:B:179:GLU:HG3	1.79	0.83
1:A:217:MET:CE	1:A:303:LEU:HB3	2.09	0.82
1:A:130:LEU:HD22	1:A:130:LEU:H	1.43	0.81
1:B:186:MET:CE	1:B:189:ARG:HD3	2.11	0.80
1:A:217:MET:HE2	1:A:305:ALA:HB2	1.65	0.78
1:A:92:ASP:OD1	1:A:95:HIS:HD2	1.66	0.78
1:B:186:MET:HE3	1:B:189:ARG:HD3	1.62	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:GLU:HB3	6:A:2:HOH:O	1.84	0.77
1:A:328:PRO:O	1:A:329:LYS:HD2	1.84	0.77
1:B:493:HIS:HD2	1:B:495:TRP:CD1	2.03	0.77
1:B:271:ILE:HD13	1:B:278:LEU:HD11	1.66	0.77
1:A:257:GLN:HE21	1:A:260:ARG:HH11	1.31	0.76
1:B:343:LEU:HD11	1:B:364:ASN:ND2	2.00	0.76
1:B:217:MET:HG2	1:B:241:PHE:CE2	2.21	0.76
1:B:441:MET:CE	1:B:472:GLN:HG2	2.16	0.75
1:B:228:ALA:HB1	1:B:364:ASN:ND2	2.01	0.75
1:B:221:ILE:HG21	1:B:301:LEU:HD21	1.67	0.74
1:B:252:ARG:NH2	1:B:489:PRO:HD3	2.03	0.73
1:A:221:ILE:O	1:A:225:ILE:HG13	1.88	0.73
1:B:116:PRO:HG2	1:B:119:LEU:HB2	1.71	0.73
1:B:302:VAL:C	1:B:303:LEU:HD12	2.08	0.73
1:A:141:ILE:HD11	1:A:163:VAL:HG21	1.69	0.73
1:A:305:ALA:O	1:A:307:GLY:N	2.21	0.72
1:B:272:ARG:HG2	1:B:272:ARG:HH11	1.55	0.72
1:A:195:ILE:HG12	1:A:458:LEU:HD23	1.71	0.72
1:B:263:GLY:O	1:B:278:LEU:HD23	1.90	0.72
1:B:410:THR:O	1:B:414:VAL:HG13	1.90	0.72
1:A:393:MET:CB	1:A:395:LEU:HD22	2.19	0.72
1:B:305:ALA:O	1:B:307:GLY:N	2.23	0.71
1:B:175:LEU:CD2	1:B:356:LEU:HD12	2.20	0.71
1:A:241:PHE:HB3	1:A:242:PRO:HD2	1.73	0.70
1:A:410:THR:O	1:A:414:VAL:HG23	1.92	0.70
1:A:130:LEU:CD2	1:A:130:LEU:H	2.04	0.70
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.27	0.70
1:B:132:GLU:O	1:B:135:PRO:HD2	1.92	0.69
1:A:386:LEU:HD21	1:A:409:VAL:HG23	1.74	0.69
1:B:110:LEU:O	1:B:112:SER:N	2.25	0.69
1:A:159:ARG:O	1:A:163:VAL:HG23	1.93	0.69
1:B:285:ILE:HD11	1:B:291:PRO:HB3	1.74	0.69
1:A:330:TYR:HB3	1:A:332:TRP:CE2	2.27	0.68
1:A:301:LEU:HB3	1:A:303:LEU:HD11	1.75	0.68
1:A:217:MET:HE1	1:A:303:LEU:HB3	1.76	0.68
1:B:152:LYS:HD2	1:B:155:GLU:OE2	1.94	0.68
1:B:164:THR:O	1:B:168:GLU:HG3	1.93	0.67
1:A:333:PHE:HA	1:A:336:LEU:HD13	1.73	0.67
1:B:241:PHE:HB3	1:B:242:PRO:HD2	1.76	0.67
1:A:301:LEU:HB3	1:A:303:LEU:CD1	2.24	0.67
1:B:441:MET:HE3	1:B:472:GLN:HG2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:MET:O	1:A:442:GLN:HG3	1.95	0.66
1:A:116:PRO:HG2	1:A:119:LEU:HB2	1.76	0.66
1:A:387:GLU:OE1	1:A:397:THR:HG21	1.96	0.66
1:A:251:PHE:O	1:A:360:ALA:HB2	1.96	0.66
1:A:274:ASP:OD1	1:A:276:ALA:HB3	1.93	0.66
1:A:417:LEU:HD21	1:A:429:ASP:HB3	1.76	0.66
1:A:445:TYR:HA	1:A:450:GLY:H	1.60	0.65
1:A:303:LEU:N	1:A:303:LEU:CD1	2.59	0.65
1:A:199:GLN:HG3	2:A:901:HEM:HBB1	1.77	0.65
1:A:153:ILE:O	1:A:157:LEU:HD13	1.95	0.65
1:A:438:MET:HG3	1:A:468:PRO:HB2	1.78	0.65
1:A:386:LEU:HB2	6:A:18:HOH:O	1.97	0.65
1:B:210:ASN:HD22	1:B:211:CYS:N	1.94	0.65
1:A:330:TYR:HD1	1:A:330:TYR:H	1.40	0.65
1:B:386:LEU:HD12	1:B:404:TRP:CZ3	2.31	0.65
1:A:453:ALA:HB1	1:A:458:LEU:CD1	2.27	0.65
1:A:92:ASP:OD1	1:A:95:HIS:CD2	2.49	0.65
1:B:199:GLN:HG3	2:B:901:HEM:HBB1	1.79	0.64
1:B:163:VAL:O	1:B:167:ILE:HG13	1.97	0.64
1:B:467:THR:CG2	1:B:469:VAL:HG22	2.27	0.64
1:B:464:GLY:O	1:B:467:THR:HB	1.98	0.64
1:B:333:PHE:HA	1:B:336:LEU:HD13	1.79	0.64
1:B:193:ARG:NH1	1:B:485:TYR:OH	2.27	0.64
1:A:262:ALA:HB2	1:A:299:LEU:HD23	1.78	0.64
1:A:380:THR:HG22	1:A:384:ASN:ND2	2.13	0.64
1:B:134:LEU:O	1:B:138:ILE:HG13	1.98	0.64
1:B:292:ARG:HG2	1:B:292:ARG:HH11	1.63	0.63
1:A:163:VAL:HG13	1:A:173:TYR:CD2	2.33	0.63
1:A:343:LEU:HD12	1:A:344:PRO:HD2	1.80	0.63
1:B:139:GLU:HG3	1:B:140:PHE:N	2.12	0.63
1:A:230:ASN:HB3	1:A:233:ASN:O	1.97	0.63
1:B:301:LEU:HD13	1:B:315:ILE:HD11	1.80	0.63
1:B:266:MET:HB3	1:B:267:PRO:HD2	1.79	0.63
1:A:252:ARG:HD2	1:A:359:PRO:O	1.97	0.63
1:A:350:LEU:HD21	1:A:357:GLU:HB2	1.80	0.63
1:A:386:LEU:HD11	1:A:405:LYS:HA	1.81	0.63
1:A:453:ALA:HB1	1:A:458:LEU:HD12	1.81	0.63
1:B:144:TYR:CE1	1:B:179:GLU:HG2	2.34	0.63
1:B:149:LYS:HG2	1:B:150:GLU:HG2	1.80	0.63
1:A:228:ALA:HB1	1:A:364:ASN:ND2	2.14	0.62
1:B:441:MET:HE1	1:B:472:GLN:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:SER:HA	1:A:481:PRO:C	2.18	0.62
1:A:459:VAL:HG22	1:A:469:VAL:HG23	1.81	0.62
1:B:316:PRO:HB2	1:B:319:LEU:HD12	1.80	0.62
1:B:380:THR:HG22	1:B:384:ASN:HD21	1.63	0.62
1:A:252:ARG:HD3	1:A:359:PRO:HB2	1.81	0.62
1:B:350:LEU:HD21	1:B:357:GLU:HB2	1.82	0.62
1:A:252:ARG:HH21	1:A:489:PRO:HD3	1.64	0.61
1:B:417:LEU:HD21	1:B:429:ASP:HB3	1.81	0.61
1:B:453:ALA:HB1	1:B:458:LEU:CD1	2.30	0.61
1:A:258:LEU:HB2	1:A:345:ALA:HB3	1.80	0.61
1:A:257:GLN:NE2	1:A:260:ARG:HD3	2.15	0.61
1:A:350:LEU:HD12	1:A:486:GLN:OE1	1.99	0.61
1:B:253:LEU:HD21	1:B:362:PRO:HG3	1.81	0.61
1:B:301:LEU:HG	1:B:303:LEU:HD11	1.81	0.61
1:A:333:PHE:O	1:A:336:LEU:HB2	2.00	0.61
1:A:110:LEU:O	1:A:112:SER:N	2.34	0.61
1:A:95:HIS:O	1:A:98:ALA:HB2	2.01	0.61
1:A:332:TRP:O	1:A:335:GLU:HB2	2.01	0.61
1:A:123:PRO:HD3	1:A:487:ILE:HD12	1.83	0.61
1:B:217:MET:HA	1:B:241:PHE:HE2	1.64	0.61
1:A:496:GLN:N	1:A:496:GLN:HE21	1.99	0.60
1:B:285:ILE:HD12	1:B:291:PRO:HD3	1.82	0.60
1:B:380:THR:HA	1:B:384:ASN:ND2	2.16	0.60
1:A:262:ALA:HB2	1:A:299:LEU:HD21	1.80	0.60
1:A:466:ILE:O	1:A:466:ILE:HG22	2.02	0.60
1:A:133:LEU:HD11	1:A:172:THR:HA	1.82	0.60
1:A:224:HIS:ND1	1:A:239:THR:HG22	2.17	0.60
1:A:266:MET:CG	1:A:272:ARG:HG3	2.32	0.60
1:B:350:LEU:HD23	1:B:350:LEU:C	2.22	0.60
1:A:285:ILE:HD12	1:A:291:PRO:HD3	1.84	0.60
1:A:380:THR:HG22	1:A:384:ASN:HD21	1.65	0.60
1:B:493:HIS:HD2	1:B:495:TRP:NE1	1.99	0.60
1:B:438:MET:HE3	1:B:469:VAL:CG1	2.17	0.59
1:A:262:ALA:CB	1:A:299:LEU:HD21	2.31	0.59
1:A:400:LEU:HD23	6:A:55:HOH:O	2.00	0.59
1:A:130:LEU:HD22	1:A:130:LEU:N	2.16	0.59
1:A:290:LYS:HE2	6:A:46:HOH:O	2.02	0.59
1:B:284:CYS:SG	1:B:300:PRO:HG2	2.43	0.59
1:B:296:PHE:CD2	1:B:339:LYS:HG2	2.38	0.59
1:B:349:MET:HE2	1:B:483:TYR:HB3	1.84	0.59
1:B:133:LEU:HD12	1:B:167:ILE:HG21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:PRO:HG2	1:B:268:ASP:OD1	2.03	0.59
1:B:350:LEU:HD23	1:B:351:LEU:O	2.03	0.59
1:B:163:VAL:HG12	1:B:167:ILE:CD1	2.29	0.58
1:B:128:THR:HG23	6:B:40:HOH:O	2.01	0.58
1:B:287:LEU:HD21	1:B:495:TRP:HH2	1.69	0.58
1:A:496:GLN:N	1:A:496:GLN:NE2	2.52	0.58
1:A:84:TRP:CE2	1:A:114:MET:HG3	2.38	0.58
1:B:224:HIS:HE1	1:B:238:ILE:HA	1.67	0.58
1:B:426:THR:HG22	1:B:427:ILE:N	2.19	0.58
1:B:478:VAL:O	1:B:479:LEU:HD23	2.03	0.58
1:B:380:THR:HG22	1:B:384:ASN:ND2	2.17	0.58
1:A:346:VAL:HG22	5:A:1:MPW:H14	1.86	0.58
1:A:346:VAL:HB	1:A:363:PHE:CE1	2.39	0.58
1:B:493:HIS:CD2	1:B:495:TRP:CD1	2.88	0.58
1:A:296:PHE:CE2	1:A:339:LYS:HG2	2.39	0.58
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.39	0.57
1:A:244:ARG:HD2	1:A:357:GLU:OE2	2.03	0.57
1:B:375:ARG:NH1	1:B:379:ASP:OD2	2.37	0.57
1:B:380:THR:HA	1:B:384:ASN:HD22	1.69	0.57
1:B:110:LEU:N	1:B:110:LEU:HD22	2.19	0.57
1:B:134:LEU:CD1	1:B:138:ILE:HD11	2.34	0.57
1:B:186:MET:HE1	1:B:189:ARG:HD3	1.86	0.57
1:B:188:TRP:CZ3	1:B:200:TRP:HA	2.39	0.57
1:B:181:ILE:HG22	1:B:182:PHE:N	2.20	0.57
1:B:197:ARG:NH2	1:B:452:PRO:O	2.38	0.57
2:A:901:HEM:HBA1	3:A:902:H4B:HN22	1.69	0.57
1:B:445:TYR:HA	1:B:450:GLY:H	1.69	0.57
1:B:175:LEU:HD23	1:B:356:LEU:CD1	2.31	0.57
1:B:262:ALA:HB2	1:B:299:LEU:CD2	2.34	0.57
2:A:901:HEM:HMC2	2:A:901:HEM:HBC2	1.86	0.57
1:A:434:SER:CB	1:A:467:THR:HG23	2.34	0.57
1:B:252:ARG:HH11	1:B:252:ARG:HG3	1.68	0.57
1:B:464:GLY:O	1:B:467:THR:N	2.35	0.57
1:A:303:LEU:N	1:A:303:LEU:HD12	2.20	0.57
1:B:480:SER:HA	1:B:481:PRO:C	2.25	0.57
1:B:77:GLN:HE21	1:B:77:GLN:HA	1.69	0.57
1:A:454:ASP:O	1:A:455:TRP:C	2.42	0.56
1:A:180:LEU:HD22	1:A:184:THR:HG23	1.87	0.56
1:B:389:VAL:O	1:B:393:MET:HG3	2.06	0.56
1:A:346:VAL:CG1	1:A:349:MET:HG3	2.35	0.56
1:A:120:THR:HG23	1:A:486:GLN:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:PHE:N	1:B:148:PHE:CD1	2.73	0.56
1:B:191:ALA:O	1:B:197:ARG:NH1	2.38	0.56
1:B:387:GLU:HG3	1:B:397:THR:HG21	1.87	0.56
1:B:289:TRP:CG	1:B:300:PRO:HG3	2.40	0.56
1:B:83:ASN:O	1:B:85:GLY:N	2.39	0.56
1:A:198:ILE:HB	1:A:440:HIS:HB2	1.88	0.56
1:B:289:TRP:CD1	1:B:300:PRO:HG3	2.40	0.56
1:B:350:LEU:HD23	1:B:351:LEU:C	2.25	0.56
1:A:165:LYS:O	1:A:169:THR:OG1	2.22	0.56
1:A:386:LEU:HD12	1:A:404:TRP:CZ3	2.41	0.56
1:B:132:GLU:C	1:B:135:PRO:HD2	2.25	0.56
1:B:459:VAL:HG22	1:B:469:VAL:HG23	1.87	0.56
1:B:264:TYR:CE1	1:B:293:TYR:HA	2.41	0.56
1:B:385:ILE:O	1:B:389:VAL:HG23	2.06	0.56
1:A:397:THR:O	1:A:397:THR:HG22	2.06	0.55
1:A:242:PRO:HG2	1:A:251:PHE:CE1	2.41	0.55
1:B:145:TYR:HE2	1:B:159:ARG:HG2	1.71	0.55
1:B:258:LEU:HB2	1:B:345:ALA:HB3	1.88	0.55
1:B:245:SER:HA	6:B:75:HOH:O	2.05	0.55
1:A:99:THR:HG22	1:A:100:SER:N	2.19	0.55
1:A:236:SER:OG	1:A:365:GLY:HA2	2.07	0.55
1:B:485:TYR:HA	6:B:61:HOH:O	2.06	0.55
1:A:110:LEU:HD22	1:A:110:LEU:N	2.22	0.55
1:B:177:LEU:O	1:B:181:ILE:HD13	2.06	0.55
1:B:467:THR:HG22	1:B:469:VAL:HG22	1.87	0.55
1:A:138:ILE:HG22	1:A:142:ASN:ND2	2.17	0.55
1:B:309:ASP:HB3	1:B:310:PRO:HD2	1.89	0.55
1:B:397:THR:HG22	1:B:397:THR:O	2.07	0.55
1:A:332:TRP:CZ3	1:A:392:ARG:HB2	2.42	0.55
1:B:188:TRP:CD2	1:B:200:TRP:HA	2.42	0.55
1:B:370:THR:HA	1:B:374:VAL:HG23	1.88	0.55
1:B:78:TYR:CD1	1:B:78:TYR:C	2.80	0.55
1:A:145:TYR:HE2	1:A:159:ARG:HG2	1.71	0.54
1:A:217:MET:HE1	1:A:304:GLN:N	2.21	0.54
1:A:242:PRO:HB2	1:A:251:PHE:CD1	2.41	0.54
1:A:252:ARG:NH2	1:A:489:PRO:HD3	2.22	0.54
1:B:192:PRO:HA	1:B:452:PRO:O	2.06	0.54
1:B:186:MET:HE1	1:B:189:ARG:HH11	1.71	0.54
1:A:348:ASN:HD22	1:A:348:ASN:C	2.09	0.54
1:A:144:TYR:O	1:A:147:SER:HB3	2.08	0.54
1:A:210:ASN:O	1:A:211:CYS:O	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:PHE:HB3	1:A:242:PRO:HD3	1.87	0.54
1:A:217:MET:HE3	1:A:303:LEU:HB3	1.87	0.54
1:A:99:THR:CG2	1:A:100:SER:N	2.70	0.54
1:B:99:THR:O	1:B:100:SER:O	2.26	0.54
1:A:266:MET:HB2	1:A:270:THR:OG1	2.07	0.54
1:A:375:ARG:HB3	1:A:375:ARG:NH1	2.23	0.54
1:B:244:ARG:NH1	1:B:357:GLU:OE2	2.40	0.54
1:A:217:MET:HA	1:A:241:PHE:HE2	1.72	0.54
1:A:386:LEU:HD21	1:A:409:VAL:CG2	2.38	0.54
1:A:387:GLU:HG3	1:A:388:GLU:N	2.23	0.54
1:A:439:LYS:HG3	1:A:443:ASN:HD21	1.73	0.53
1:B:330:TYR:HD2	1:B:332:TRP:HE1	1.55	0.53
1:B:417:LEU:O	1:B:421:GLN:HB2	2.08	0.53
1:A:332:TRP:CE3	1:A:392:ARG:HD2	2.43	0.53
1:B:408:ALA:O	1:B:411:GLU:N	2.42	0.53
1:A:132:GLU:C	1:A:135:PRO:HD2	2.28	0.53
1:A:173:TYR:CE1	1:A:356:LEU:HD11	2.44	0.53
1:B:140:PHE:CE2	1:B:175:LEU:HD11	2.42	0.53
1:B:285:ILE:CD1	1:B:291:PRO:HD3	2.38	0.53
1:A:420:PHE:CG	1:A:427:ILE:HD12	2.44	0.53
1:A:488:GLU:HG3	6:A:29:HOH:O	2.07	0.53
1:A:292:ARG:HG2	1:A:292:ARG:HH11	1.74	0.53
1:A:380:THR:HA	1:A:384:ASN:ND2	2.23	0.53
1:A:445:TYR:O	1:A:449:GLY:HA2	2.08	0.53
1:A:172:THR:OG1	1:A:173:TYR:N	2.41	0.53
1:A:393:MET:CE	1:A:411:GLU:HG3	2.39	0.53
1:B:241:PHE:HB3	1:B:242:PRO:HD3	1.89	0.53
1:A:257:GLN:HE21	1:A:260:ARG:NH1	2.01	0.53
1:A:327:HIS:ND1	1:A:328:PRO:HD2	2.24	0.53
1:A:338:LEU:HB2	6:A:62:HOH:O	2.09	0.52
1:A:164:THR:O	1:A:168:GLU:HG2	2.09	0.52
1:B:194:CYS:O	1:B:197:ARG:HG3	2.10	0.52
1:B:252:ARG:NH1	1:B:252:ARG:HG3	2.24	0.52
1:A:199:GLN:O	1:A:201:SER:N	2.42	0.52
1:A:218:PHE:CD1	1:A:313:PHE:HB3	2.45	0.52
1:A:437:PHE:O	1:A:440:HIS:HB3	2.10	0.52
1:B:252:ARG:HD3	1:B:359:PRO:HB2	1.91	0.52
1:A:368:MET:O	1:A:369:GLY:C	2.47	0.52
1:A:467:THR:CG2	1:A:469:VAL:HG22	2.40	0.52
1:B:274:ASP:OD1	1:B:276:ALA:HB3	2.10	0.52
1:B:292:ARG:HG2	1:B:292:ARG:NH1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:HIS:C	1:B:306:ASP:O	2.47	0.52
1:B:177:LEU:HD13	1:B:177:LEU:O	2.10	0.51
1:B:210:ASN:H	1:B:210:ASN:ND2	2.08	0.51
1:B:333:PHE:O	1:B:336:LEU:HB2	2.10	0.51
1:A:343:LEU:HD11	1:A:364:ASN:HD22	1.75	0.51
1:B:199:GLN:O	1:B:201:SER:N	2.44	0.51
1:B:268:ASP:N	1:B:268:ASP:OD1	2.35	0.51
1:A:332:TRP:CH2	1:A:392:ARG:HB2	2.45	0.51
1:B:264:TYR:CZ	1:B:293:TYR:HA	2.46	0.51
1:B:296:PHE:CE2	1:B:339:LYS:HG2	2.45	0.51
1:B:368:MET:O	1:B:369:GLY:C	2.47	0.51
1:A:467:THR:HG22	1:A:469:VAL:HG22	1.92	0.51
1:B:138:ILE:HG23	1:B:160:LEU:CD2	2.40	0.51
1:A:266:MET:SD	1:A:272:ARG:HD2	2.51	0.51
1:A:346:VAL:HG11	1:A:349:MET:HG3	1.92	0.51
1:B:298:VAL:HG21	1:B:320:VAL:HG11	1.92	0.51
1:B:171:GLY:O	1:B:172:THR:HB	2.11	0.51
1:B:251:PHE:O	1:B:360:ALA:HB2	2.11	0.51
1:A:111:GLY:C	1:A:113:ILE:H	2.15	0.51
1:A:480:SER:HA	1:A:481:PRO:O	2.10	0.51
1:A:199:GLN:HG3	2:A:901:HEM:CBB	2.41	0.51
1:B:224:HIS:HE1	1:B:238:ILE:CA	2.23	0.51
1:B:134:LEU:HD12	1:B:138:ILE:HD11	1.92	0.51
1:B:374:VAL:O	1:B:378:CYS:HB2	2.10	0.51
1:A:163:VAL:O	1:A:167:ILE:HG13	2.11	0.51
1:B:182:PHE:O	1:B:186:MET:HB2	2.11	0.51
1:A:444:GLU:HG2	1:A:451:CYS:HB2	1.93	0.50
1:A:412:ILE:O	1:A:415:ALA:HB3	2.11	0.50
1:B:387:GLU:HB3	6:B:8:HOH:O	2.10	0.50
1:B:133:LEU:C	1:B:133:LEU:HD13	2.31	0.50
1:B:228:ALA:CB	1:B:364:ASN:HD21	2.18	0.50
1:B:330:TYR:HB3	1:B:332:TRP:NE1	2.27	0.50
1:A:217:MET:HA	1:A:241:PHE:CE2	2.47	0.50
1:B:180:LEU:HD21	1:B:240:VAL:HG11	1.93	0.50
1:A:316:PRO:O	1:A:318:ASP:N	2.45	0.50
1:B:175:LEU:HD12	1:B:179:GLU:HB2	1.93	0.50
1:B:177:LEU:HD13	1:B:177:LEU:C	2.32	0.50
1:A:154:GLU:HG2	1:A:155:GLU:H	1.77	0.50
1:A:389:VAL:O	1:A:393:MET:HG3	2.11	0.50
1:B:257:GLN:NE2	5:B:1:MPW:N2	2.60	0.50
1:B:350:LEU:HD23	1:B:351:LEU:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ARG:HG2	1:B:89:ILE:HG21	1.93	0.49
1:B:466:ILE:O	1:B:466:ILE:HG22	2.12	0.49
1:B:96:HIS:C	1:B:98:ALA:H	2.14	0.49
1:B:330:TYR:HD2	1:B:332:TRP:NE1	2.09	0.49
1:A:438:MET:HA	1:A:438:MET:CE	2.41	0.49
1:A:188:TRP:CZ3	1:A:200:TRP:HA	2.47	0.49
1:A:230:ASN:HB2	1:A:235:ARG:HE	1.77	0.49
1:A:263:GLY:O	1:A:278:LEU:HD23	2.11	0.49
1:A:294:GLY:N	1:A:297:ASP:OD2	2.46	0.49
1:A:369:GLY:O	1:A:371:GLU:N	2.45	0.49
1:A:123:PRO:CD	1:A:487:ILE:HD12	2.43	0.48
1:B:136:HIS:O	1:B:139:GLU:HB3	2.13	0.48
1:B:173:TYR:OH	1:B:354:GLY:HA3	2.12	0.48
1:B:453:ALA:HB1	1:B:458:LEU:HD12	1.95	0.48
1:A:385:ILE:HD11	1:A:412:ILE:HD13	1.95	0.48
1:B:332:TRP:CZ3	1:B:392:ARG:HB2	2.48	0.48
1:B:223:ARG:HD3	6:B:14:HOH:O	2.13	0.48
1:A:272:ARG:HG2	1:A:272:ARG:HH11	1.77	0.48
1:B:128:THR:OG1	1:B:133:LEU:HB2	2.13	0.48
1:B:217:MET:HG2	1:B:241:PHE:HE2	1.78	0.48
1:B:438:MET:O	1:B:442:GLN:HG3	2.14	0.48
1:B:303:LEU:CD1	1:B:303:LEU:N	2.77	0.48
1:A:124:ARG:NH1	1:A:128:THR:OG1	2.46	0.48
1:A:266:MET:HG3	1:A:272:ARG:HG3	1.96	0.48
1:A:272:ARG:HG2	1:A:272:ARG:NH1	2.29	0.48
1:A:292:ARG:O	1:A:293:TYR:C	2.52	0.48
1:A:83:ASN:O	1:A:87:GLY:N	2.47	0.48
1:B:285:ILE:CD1	1:B:291:PRO:HB3	2.42	0.48
1:A:330:TYR:CD1	1:A:330:TYR:N	2.75	0.48
1:A:260:ARG:HH21	1:A:276:ALA:HB3	1.78	0.48
1:B:386:LEU:HD12	1:B:404:TRP:HZ3	1.79	0.48
1:A:253:LEU:HD12	1:A:253:LEU:N	2.28	0.47
1:B:217:MET:HA	1:B:241:PHE:CE2	2.46	0.47
1:A:234:ILE:HG22	1:A:235:ARG:N	2.29	0.47
1:B:215:GLN:OE1	1:B:219:GLN:NE2	2.47	0.47
1:B:77:GLN:NE2	1:B:77:GLN:HA	2.29	0.47
1:A:210:ASN:O	1:A:211:CYS:C	2.53	0.47
1:A:417:LEU:O	1:A:421:GLN:HB2	2.15	0.47
1:A:493:HIS:CG	1:A:494:ILE:H	2.33	0.47
1:B:223:ARG:HG3	1:B:223:ARG:HH11	1.79	0.47
1:B:361:CYS:SG	1:B:361:CYS:O	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:THR:HG21	1:B:469:VAL:HG22	1.95	0.47
1:A:333:PHE:CD1	1:A:336:LEU:HD22	2.50	0.47
1:A:291:PRO:C	1:A:293:TYR:H	2.18	0.47
1:B:133:LEU:HD12	1:B:167:ILE:CG2	2.44	0.47
1:B:221:ILE:HD12	1:B:303:LEU:HD21	1.97	0.47
1:B:272:ARG:HG2	1:B:272:ARG:NH1	2.24	0.47
1:A:380:THR:HA	1:A:384:ASN:HD22	1.78	0.47
1:A:395:LEU:N	1:A:395:LEU:HD13	2.29	0.46
1:A:445:TYR:O	1:A:449:GLY:N	2.49	0.46
1:B:153:ILE:O	1:B:157:LEU:HD13	2.13	0.46
1:A:274:ASP:O	1:A:276:ALA:N	2.48	0.46
1:A:320:VAL:O	1:A:320:VAL:HG12	2.14	0.46
1:A:333:PHE:O	1:A:336:LEU:HD13	2.16	0.46
2:A:901:HEM:CMC	2:A:901:HEM:HBC2	2.45	0.46
1:B:130:LEU:HD11	1:B:134:LEU:HD23	1.96	0.46
1:B:303:LEU:HD12	1:B:303:LEU:N	2.29	0.46
1:B:80:ARG:HG2	1:B:89:ILE:CG2	2.45	0.46
1:A:253:LEU:CD1	1:A:360:ALA:HB1	2.45	0.46
1:A:268:ASP:OD1	1:A:268:ASP:N	2.40	0.46
1:A:78:TYR:CD1	1:A:78:TYR:C	2.88	0.46
1:B:250:ASP:N	1:B:306:ASP:O	2.48	0.46
1:B:328:PRO:HD3	1:B:418:HIS:ND1	2.31	0.46
1:B:372:ILE:HA	1:B:376:ASP:OD2	2.16	0.46
1:A:444:GLU:HG3	1:A:450:GLY:O	2.14	0.46
1:B:130:LEU:HD13	1:B:134:LEU:HB2	1.98	0.46
1:B:89:ILE:HG22	1:B:90:LEU:N	2.31	0.46
1:B:287:LEU:HD11	1:B:310:PRO:CG	2.45	0.46
1:A:180:LEU:CD2	1:A:184:THR:HG23	2.46	0.46
1:A:95:HIS:O	1:A:98:ALA:CB	2.63	0.46
1:B:177:LEU:CD1	1:B:181:ILE:HD13	2.36	0.46
1:B:408:ALA:O	1:B:409:VAL:C	2.54	0.46
1:A:171:GLY:C	1:A:172:THR:HG22	2.36	0.46
1:A:251:PHE:CE2	1:A:305:ALA:HB1	2.51	0.46
1:A:344:PRO:O	1:A:344:PRO:HG2	2.16	0.46
1:B:400:LEU:O	1:B:402:SER:N	2.49	0.46
1:B:238:ILE:HG13	1:B:362:PRO:O	2.16	0.46
1:B:121:ARG:HD3	1:B:121:ARG:HA	1.63	0.45
1:B:99:THR:CG2	1:B:100:SER:N	2.78	0.45
1:A:321:LEU:HD12	1:A:322:GLU:N	2.31	0.45
1:B:272:ARG:NH1	1:B:295:ARG:HG3	2.32	0.45
1:A:267:PRO:HB3	1:B:293:TYR:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:GLU:HG2	1:B:165:LYS:HE3	1.98	0.45
1:B:194:CYS:HB2	2:B:901:HEM:ND	2.31	0.45
1:B:210:ASN:HD22	1:B:211:CYS:H	1.63	0.45
1:B:267:PRO:C	1:B:269:GLY:H	2.19	0.45
1:B:95:HIS:O	1:B:98:ALA:HB2	2.15	0.45
1:A:228:ALA:HB1	1:A:364:ASN:HD21	1.79	0.45
1:A:333:PHE:CE2	1:A:415:ALA:HB1	2.52	0.45
1:B:287:LEU:HD21	1:B:495:TRP:CH2	2.50	0.45
1:A:195:ILE:HD12	1:A:368:MET:HE1	1.94	0.45
1:A:236:SER:HA	1:A:364:ASN:O	2.16	0.45
1:B:110:LEU:H	1:B:110:LEU:HD22	1.81	0.45
1:A:134:LEU:HB3	1:A:135:PRO:HD3	1.99	0.45
1:B:445:TYR:O	1:B:449:GLY:HA2	2.17	0.45
1:A:154:GLU:HG2	1:A:155:GLU:N	2.32	0.45
1:B:251:PHE:CE1	1:B:306:ASP:HA	2.52	0.45
1:A:253:LEU:HD12	1:A:253:LEU:H	1.82	0.45
1:A:249:HIS:C	1:A:306:ASP:O	2.55	0.45
1:B:210:ASN:ND2	1:B:210:ASN:N	2.65	0.45
1:A:374:VAL:HG11	1:A:462:VAL:HG13	1.99	0.44
1:A:121:ARG:HD3	1:A:121:ARG:HA	1.85	0.44
1:B:177:LEU:HD23	1:B:207:ASP:OD2	2.18	0.44
1:B:261:TYR:HA	1:B:297:ASP:O	2.17	0.44
1:A:386:LEU:HD13	1:A:386:LEU:O	2.17	0.44
1:B:229:THR:O	1:B:230:ASN:C	2.55	0.44
1:B:242:PRO:HG2	1:B:251:PHE:CZ	2.52	0.44
1:A:267:PRO:C	1:A:269:GLY:H	2.21	0.44
1:A:262:ALA:CB	1:A:299:LEU:CD2	2.82	0.44
1:A:417:LEU:HD21	1:A:429:ASP:CB	2.46	0.44
1:B:233:ASN:C	1:B:233:ASN:HD22	2.20	0.44
1:B:287:LEU:CD1	1:B:310:PRO:HG2	2.48	0.44
1:B:454:ASP:O	1:B:455:TRP:C	2.55	0.44
1:B:86:SER:C	1:B:88:GLU:H	2.21	0.44
1:A:402:SER:OG	1:A:404:TRP:HD1	2.00	0.44
1:B:301:LEU:HB3	1:B:303:LEU:CD1	2.47	0.44
1:B:353:VAL:O	1:B:354:GLY:C	2.55	0.44
1:A:272:ARG:NH2	1:A:295:ARG:HG3	2.33	0.44
1:A:333:PHE:CE2	1:A:415:ALA:CB	3.01	0.44
1:B:482:PHE:HB3	1:B:484:TYR:CE1	2.52	0.44
1:A:393:MET:HE3	1:A:411:GLU:HG3	1.99	0.44
1:B:224:HIS:O	1:B:225:ILE:C	2.56	0.44
1:A:309:ASP:HB3	1:A:310:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ASP:HB2	1:A:382:ARG:HG2	2.00	0.44
1:B:239:THR:CG2	1:B:362:PRO:HG2	2.48	0.44
1:A:149:LYS:HG2	1:A:150:GLU:HG2	1.99	0.44
1:A:257:GLN:HE22	1:A:260:ARG:HD3	1.83	0.43
1:B:348:ASN:C	1:B:348:ASN:HD22	2.20	0.43
1:B:342:ALA:HB1	1:B:425:VAL:HG11	2.00	0.43
1:A:210:ASN:C	1:A:211:CYS:O	2.57	0.43
1:A:167:ILE:C	1:A:169:THR:H	2.22	0.43
1:A:196:GLY:O	1:A:198:ILE:N	2.52	0.43
1:B:217:MET:O	1:B:220:HIS:N	2.51	0.43
1:B:242:PRO:HG2	1:B:251:PHE:CE1	2.53	0.43
1:B:246:ASP:OD2	1:B:248:LYS:HB2	2.18	0.43
1:B:381:GLN:O	1:B:382:ARG:HD2	2.19	0.43
1:A:195:ILE:HD12	1:A:368:MET:HE2	1.97	0.43
1:A:248:LYS:HE3	1:A:494:ILE:CD1	2.48	0.43
1:B:130:LEU:CD1	1:B:134:LEU:HD23	2.48	0.43
1:A:206:PHE:HB2	1:A:239:THR:HA	2.01	0.43
1:A:211:CYS:SG	1:A:216:GLU:HB3	2.58	0.43
1:A:301:LEU:HB3	1:A:303:LEU:HD13	1.98	0.43
1:B:301:LEU:HB3	1:B:303:LEU:HD11	2.01	0.43
1:A:218:PHE:CE1	1:A:313:PHE:HB3	2.53	0.43
1:A:343:LEU:HD11	1:A:364:ASN:ND2	2.33	0.43
1:B:285:ILE:HD12	1:B:291:PRO:CD	2.48	0.43
1:A:198:ILE:HA	1:A:440:HIS:ND1	2.34	0.43
1:A:253:LEU:HD22	1:A:347:ALA:HB1	2.01	0.43
1:A:261:TYR:HA	1:A:297:ASP:O	2.19	0.43
1:A:333:PHE:CA	1:A:336:LEU:HD13	2.46	0.43
1:B:181:ILE:HD12	1:B:205:VAL:HG11	2.00	0.43
1:B:333:PHE:O	1:B:336:LEU:HD13	2.19	0.43
1:B:332:TRP:O	1:B:335:GLU:HB2	2.19	0.43
1:A:244:ARG:HG3	1:A:250:ASP:OD1	2.18	0.43
1:A:375:ARG:NH1	1:A:379:ASP:OD2	2.52	0.43
1:A:493:HIS:CG	1:A:494:ILE:N	2.87	0.43
1:B:138:ILE:HG23	1:B:160:LEU:HD22	2.01	0.43
1:B:267:PRO:HG2	1:B:268:ASP:H	1.84	0.43
1:A:386:LEU:CB	6:A:18:HOH:O	2.61	0.42
1:B:291:PRO:HG2	1:B:293:TYR:CE2	2.54	0.42
1:B:320:VAL:O	1:B:320:VAL:HG12	2.19	0.42
1:B:330:TYR:CD2	1:B:332:TRP:CZ2	3.07	0.42
1:B:253:LEU:CD1	1:B:360:ALA:HB1	2.49	0.42
1:A:230:ASN:HB2	1:A:235:ARG:NE	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:PRO:HG2	1:A:268:ASP:OD1	2.19	0.42
1:A:174:GLN:HA	6:A:34:HOH:O	2.18	0.42
1:A:177:LEU:O	1:A:177:LEU:HD12	2.19	0.42
1:A:281:THR:O	1:A:282:GLN:C	2.56	0.42
1:A:289:TRP:CZ3	1:A:291:PRO:HA	2.54	0.42
1:A:346:VAL:HG12	1:A:349:MET:HG3	2.00	0.42
1:B:289:TRP:CZ3	1:B:291:PRO:HA	2.54	0.42
1:A:342:ALA:HB1	1:A:425:VAL:CG1	2.49	0.42
1:A:420:PHE:O	1:A:421:GLN:C	2.58	0.42
1:A:264:TYR:CE1	1:A:293:TYR:HA	2.54	0.42
1:A:316:PRO:HD2	1:A:319:LEU:HD12	2.02	0.42
1:A:316:PRO:CG	1:A:319:LEU:HD12	2.49	0.42
1:B:210:ASN:N	1:B:210:ASN:HD22	2.16	0.42
1:B:438:MET:HA	1:B:438:MET:HE2	2.00	0.42
1:B:455:TRP:CZ2	1:B:459:VAL:HG21	2.55	0.42
1:B:480:SER:HA	1:B:481:PRO:O	2.19	0.42
1:A:316:PRO:O	1:A:317:PRO:C	2.58	0.42
1:A:195:ILE:CD1	1:A:368:MET:CE	2.90	0.42
1:A:395:LEU:HD13	1:A:395:LEU:H	1.85	0.42
1:B:239:THR:O	1:B:239:THR:HG23	2.19	0.42
1:B:408:ALA:O	1:B:410:THR:N	2.53	0.42
1:A:242:PRO:HG2	1:A:251:PHE:CZ	2.55	0.42
1:A:280:PHE:HD2	1:A:299:LEU:HD13	1.85	0.42
1:B:426:THR:CG2	1:B:427:ILE:N	2.83	0.42
1:A:110:LEU:H	1:A:110:LEU:HD22	1.85	0.42
1:A:257:GLN:OE1	5:A:1:MPW:N2	2.53	0.42
1:B:153:ILE:HG13	1:B:153:ILE:H	1.61	0.42
1:B:264:TYR:N	1:B:264:TYR:CD1	2.88	0.42
1:B:281:THR:O	1:B:285:ILE:HG12	2.20	0.42
1:B:133:LEU:CD1	1:B:167:ILE:HG21	2.50	0.41
1:B:445:TYR:O	1:B:449:GLY:N	2.53	0.41
1:B:204:GLN:HB3	1:B:237:ALA:CB	2.49	0.41
1:A:316:PRO:HB2	1:A:319:LEU:HD12	2.03	0.41
1:A:348:ASN:C	1:A:348:ASN:ND2	2.74	0.41
1:A:464:GLY:O	1:A:467:THR:HB	2.21	0.41
1:B:165:LYS:O	1:B:169:THR:OG1	2.39	0.41
1:B:289:TRP:CE2	1:B:300:PRO:HD3	2.55	0.41
1:A:195:ILE:HD12	1:A:368:MET:HE3	1.99	0.41
1:A:445:TYR:O	1:A:449:GLY:CA	2.69	0.41
1:B:138:ILE:HG22	1:B:142:ASN:ND2	2.35	0.41
1:A:282:GLN:O	1:A:283:LEU:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:THR:HG23	1:A:468:PRO:HD2	2.02	0.41
1:A:349:MET:SD	2:A:901:HEM:HMD3	2.61	0.41
1:B:149:LYS:O	1:B:150:GLU:C	2.58	0.41
1:B:188:TRP:CZ2	2:B:901:HEM:HMC1	2.56	0.41
1:A:282:GLN:O	1:A:285:ILE:N	2.53	0.41
1:A:301:LEU:N	1:A:313:PHE:O	2.54	0.41
1:B:301:LEU:HA	1:B:301:LEU:HD12	1.71	0.41
1:A:111:GLY:O	1:A:113:ILE:N	2.53	0.41
1:A:327:HIS:ND1	1:A:328:PRO:CD	2.84	0.41
1:A:84:TRP:O	1:A:381:GLN:NE2	2.53	0.41
1:A:451:CYS:HA	1:A:452:PRO:HD2	1.88	0.41
1:B:332:TRP:CH2	1:B:392:ARG:HB2	2.55	0.41
1:B:382:ARG:HH22	5:B:1:MPW:H4	1.86	0.41
1:A:215:GLN:NE2	6:A:20:HOH:O	2.37	0.41
1:A:266:MET:SD	1:A:272:ARG:CD	3.09	0.41
1:A:195:ILE:CD1	1:A:368:MET:HE1	2.51	0.41
1:B:368:MET:HA	1:B:428:MET:O	2.21	0.41
1:A:152:LYS:O	1:A:155:GLU:N	2.53	0.41
1:B:316:PRO:HB2	1:B:319:LEU:CD1	2.49	0.41
1:B:379:ASP:HB2	1:B:382:ARG:HG2	2.03	0.41
1:B:350:LEU:CD2	1:B:351:LEU:O	2.68	0.40
1:A:145:TYR:C	1:A:147:SER:H	2.24	0.40
1:A:375:ARG:HB3	1:A:375:ARG:HH11	1.84	0.40
1:A:386:LEU:HA	1:A:386:LEU:HD22	1.84	0.40
1:B:330:TYR:HB3	1:B:332:TRP:CE2	2.56	0.40
1:B:487:ILE:O	1:B:488:GLU:C	2.59	0.40
1:A:218:PHE:CD1	1:A:313:PHE:CB	3.04	0.40
1:A:376:ASP:OD1	1:A:382:ARG:NH2	2.54	0.40
1:B:382:ARG:NH2	5:B:1:MPW:H4	2.37	0.40
1:B:228:ALA:CB	1:B:364:ASN:ND2	2.79	0.40
1:B:477:TYR:HD2	1:B:479:LEU:HD21	1.87	0.40
1:A:187:ALA:HB2	1:A:481:PRO:HB2	2.04	0.40
1:A:239:THR:O	1:A:239:THR:HG23	2.22	0.40
1:A:374:VAL:O	1:A:378:CYS:HB2	2.22	0.40
1:A:388:GLU:HA	1:A:391:ARG:HB2	2.04	0.40
1:B:199:GLN:O	1:B:200:TRP:C	2.59	0.40
1:B:225:ILE:HG13	1:B:225:ILE:H	1.71	0.40
1:B:258:LEU:HA	1:B:258:LEU:HD12	1.87	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	410/423 (97%)	311 (76%)	69 (17%)	30 (7%)	1	2
1	B	409/423 (97%)	314 (77%)	71 (17%)	24 (6%)	1	4
All	All	819/846 (97%)	625 (76%)	140 (17%)	54 (7%)	1	3

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	GLY
1	A	200	TRP
1	A	268	ASP
1	B	84	TRP
1	B	98	ALA
1	B	111	GLY
1	B	306	ASP
1	A	84	TRP
1	A	112	SER
1	A	150	GLU
1	A	153	ILE
1	A	172	THR
1	A	211	CYS
1	A	293	TYR
1	A	306	ASP
1	A	330	TYR
1	A	369	GLY
1	A	370	THR
1	A	387	GLU
1	B	197	ARG
1	B	200	TRP
1	B	211	CYS
1	B	230	ASN
1	B	268	ASP
1	B	293	TYR

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Mol	Chain	Res	Type
1	B	369	GLY
1	B	401	ALA
1	A	197	ARG
1	A	270	THR
1	A	275	ALA
1	A	455	TRP
1	B	150	GLU
1	B	379	ASP
1	A	307	GLY
1	A	423	GLN
1	B	172	THR
1	B	224	HIS
1	B	408	ALA
1	B	423	GLN
1	A	129	PRO
1	A	151	ALA
1	A	230	ASN
1	A	316	PRO
1	A	317	PRO
1	B	316	PRO
1	A	123	PRO
1	A	168	GLU
1	A	447	ALA
1	B	409	VAL
1	B	225	ILE
1	B	307	GLY
1	B	317	PRO
1	A	291	PRO
1	B	456	ILE

### 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	362/371 (98%)	339 (94%)	23 (6%)	17	45
1	B	361/371 (97%)	334 (92%)	27 (8%)	13	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	723/742 (97%)	673 (93%)	50 (7%)	15	41

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	TYR
1	A	114	MET
1	A	129	PRO
1	A	148	PHE
1	A	172	THR
1	A	180	LEU
1	A	219	GLN
1	A	231	ASN
1	A	233	ASN
1	A	239	THR
1	A	264	TYR
1	A	268	ASP
1	A	292	ARG
1	A	301	LEU
1	A	303	LEU
1	A	324	THR
1	A	330	TYR
1	A	348	ASN
1	A	386	LEU
1	A	395	LEU
1	A	406	ASP
1	A	475	LEU
1	A	496	GLN
1	B	99	THR
1	B	119	LEU
1	B	121	ARG
1	B	128	THR
1	B	130	LEU
1	B	134	LEU
1	B	139	GLU
1	B	148	PHE
1	B	169	THR
1	B	210	ASN
1	B	219	GLN
1	B	226	LEU
1	B	231	ASN
1	B	233	ASN

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Mol	Chain	Res	Type
1	B	258	LEU
1	B	264	TYR
1	B	290	LYS
1	B	292	ARG
1	B	301	LEU
1	B	303	LEU
1	B	324	THR
1	B	348	ASN
1	B	386	LEU
1	B	444	GLU
1	B	475	LEU
1	B	485	TYR
1	B	496	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	HIS
1	A	95	HIS
1	A	96	HIS
1	A	142	ASN
1	A	219	GLN
1	A	231	ASN
1	A	233	ASN
1	A	257	GLN
1	A	334	GLN
1	A	348	ASN
1	A	384	ASN
1	A	423	GLN
1	A	496	GLN
1	B	77	GLN
1	B	95	HIS
1	B	96	HIS
1	B	142	ASN
1	B	210	ASN
1	B	219	GLN
1	B	231	ASN
1	B	233	ASN
1	B	249	HIS
1	B	348	ASN
1	B	364	ASN
1	B	384	ASN

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Mol	Chain	Res	Type
1	B	493	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

7 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	$\# Z  > 2$
5	MPW	B	1	-	19,21,21	1.36	2 (10%)	22,28,28	2.46	8 (36%)
5	MPW	A	1	-	19,21,21	1.67	4 (21%)	22,28,28	2.59	9 (40%)
3	H4B	B	902	-	16,18,18	2.41	7 (43%)	11,26,26	4.19	7 (63%)
3	H4B	A	902	-	16,18,18	2.63	6 (37%)	11,26,26	4.05	7 (63%)
4	SO4	A	907	-	4,4,4	0.32	0	6,6,6	0.09	0
2	HEM	A	901	1	27,50,50	1.86	7 (25%)	17,82,82	2.36	9 (52%)
2	HEM	B	901	1	27,50,50	1.89	6 (22%)	17,82,82	2.43	9 (52%)

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
5	MPW	B	1	-	-	3/7/7/7	0/3/3/3
5	MPW	A	1	-	-	3/7/7/7	0/3/3/3
3	H4B	B	902	-	-	0/8/17/17	0/2/2/2
3	H4B	A	902	-	-	0/8/17/17	0/2/2/2
2	HEM	A	901	1	-	1/6/54/54	-
2	HEM	B	901	1	-	1/6/54/54	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	H4B	C4-N3	5.82	1.43	1.33
3	B	902	H4B	C4-N3	5.72	1.43	1.33
3	A	902	H4B	C4A-N5	5.33	1.48	1.38
3	A	902	H4B	C6-N5	4.43	1.54	1.45
3	B	902	H4B	C4A-N5	4.39	1.47	1.38
2	B	901	HEM	C3C-CAC	4.26	1.56	1.47
2	B	901	HEM	CBC-CAC	4.07	1.56	1.29
2	A	901	HEM	CBC-CAC	4.07	1.56	1.29
3	B	902	H4B	C6-N5	3.91	1.53	1.45
2	A	901	HEM	C3C-CAC	3.78	1.55	1.47
2	B	901	HEM	CBB-CAB	3.78	1.54	1.29
2	A	901	HEM	CBB-CAB	3.74	1.54	1.29
5	A	1	MPW	C5-N2	3.65	1.41	1.34
2	B	901	HEM	C3B-C2B	-3.15	1.36	1.40
2	B	901	HEM	C3C-C2C	-2.90	1.36	1.40
3	A	902	H4B	C7-N8	2.86	1.49	1.44
5	B	1	MPW	C5-N2	2.85	1.40	1.34
5	A	1	MPW	C7-C8	2.77	1.57	1.51
2	A	901	HEM	C3C-C2C	-2.71	1.36	1.40
5	B	1	MPW	C13-C11	2.60	1.43	1.38
3	A	902	H4B	C8A-N1	2.56	1.39	1.34
5	A	1	MPW	C8-N3	2.47	1.39	1.34
2	A	901	HEM	C3B-C2B	-2.45	1.37	1.40
5	A	1	MPW	C13-C11	2.41	1.43	1.38
2	B	901	HEM	C4D-C3D	2.38	1.48	1.42
3	B	902	H4B	C7-N8	2.30	1.48	1.44
3	A	902	H4B	C7-C6	2.30	1.54	1.52
3	B	902	H4B	C8A-N1	2.19	1.38	1.34
3	B	902	H4B	C7-C6	2.19	1.54	1.52
2	A	901	HEM	C4D-C3D	2.17	1.47	1.42
3	B	902	H4B	C2-N3	2.11	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	HEM	C1C-C2C	2.01	1.47	1.42

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	H4B	C4-C4A-C8A	9.43	122.94	114.57
3	A	902	H4B	C4-C4A-C8A	8.58	122.19	114.57
5	A	1	MPW	C7-C14-C6	-6.84	100.89	112.48
5	B	1	MPW	C7-C14-C6	-6.36	101.70	112.48
5	A	1	MPW	C4-N1-C5	6.15	124.19	116.60
5	B	1	MPW	C4-N1-C5	6.06	124.08	116.60
3	B	902	H4B	C4-N3-C2	5.80	125.14	115.93
3	A	902	H4B	C4-N3-C2	5.72	125.03	115.93
3	A	902	H4B	N3-C2-N1	-4.84	117.83	125.42
3	B	902	H4B	N3-C2-N1	-4.56	118.26	125.42
2	B	901	HEM	CAA-CBA-CGA	4.41	120.07	112.67
2	A	901	HEM	CAA-CBA-CGA	4.30	119.88	112.67
2	B	901	HEM	CBD-CAD-C3D	-4.27	104.61	112.48
3	B	902	H4B	C4A-C4-N3	-3.84	113.08	124.01
2	A	901	HEM	CMC-C2C-C3C	3.80	131.79	124.68
3	A	902	H4B	C2-N1-C8A	3.69	122.82	114.54
3	A	902	H4B	N2-C2-N1	3.60	122.86	117.25
2	A	901	HEM	CBD-CAD-C3D	-3.57	105.90	112.48
3	A	902	H4B	C4A-C4-N3	-3.56	113.89	124.01
3	B	902	H4B	C2-N1-C8A	3.52	122.43	114.54
2	B	901	HEM	CMC-C2C-C3C	3.46	131.15	124.68
3	B	902	H4B	N2-C2-N1	3.33	122.43	117.25
5	B	1	MPW	C12-O-C11	3.29	124.65	117.51
5	A	1	MPW	C12-O-C11	3.20	124.46	117.51
2	B	901	HEM	CMB-C2B-C3B	3.09	130.46	124.68
2	B	901	HEM	CMA-C3A-C4A	-2.95	123.93	128.46
5	B	1	MPW	C3-C4-N1	-2.94	119.44	123.94
5	A	1	MPW	C9-N3-C8	2.89	121.38	117.42
2	A	901	HEM	CMD-C2D-C3D	2.88	130.37	124.94
2	A	901	HEM	C1D-C2D-C3D	-2.84	105.02	107.00
5	A	1	MPW	C7-C8-N3	2.83	122.72	116.91
2	B	901	HEM	C1D-C2D-C3D	-2.82	105.03	107.00
5	B	1	MPW	C5-C1-N4	-2.80	105.78	109.19
5	A	1	MPW	C3-C4-N1	-2.78	119.69	123.94
3	A	902	H4B	C4A-N5-C6	-2.73	113.72	121.16
3	B	902	H4B	C4A-N5-C6	-2.71	113.79	121.16
2	A	901	HEM	CMB-C2B-C3B	2.71	129.74	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	HEM	CMA-C3A-C4A	-2.69	124.33	128.46
5	A	1	MPW	C5-C1-N4	-2.63	105.99	109.19
2	B	901	HEM	CMD-C2D-C3D	2.59	129.83	124.94
2	A	901	HEM	CMD-C2D-C1D	-2.53	124.58	128.46
2	B	901	HEM	CMA-C3A-C2A	2.47	129.60	124.94
2	A	901	HEM	CMA-C3A-C2A	2.45	129.55	124.94
5	B	1	MPW	C9-N3-C8	2.43	120.75	117.42
5	B	1	MPW	C2-C1-N4	2.21	137.19	130.78
5	A	1	MPW	C13-C8-N3	-2.21	118.66	121.78
2	B	901	HEM	CMD-C2D-C1D	-2.17	125.12	128.46
5	A	1	MPW	C2-C1-N4	2.16	137.05	130.78
5	B	1	MPW	C7-C8-N3	2.03	121.07	116.91

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1	MPW	C6-C14-C7-C8
2	A	901	HEM	C2A-CAA-CBA-CGA
2	B	901	HEM	C2A-CAA-CBA-CGA
5	B	1	MPW	C14-C7-C8-C13
5	A	1	MPW	C14-C7-C8-C13
5	B	1	MPW	C6-C14-C7-C8
5	B	1	MPW	C14-C7-C8-N3
5	A	1	MPW	C14-C7-C8-N3

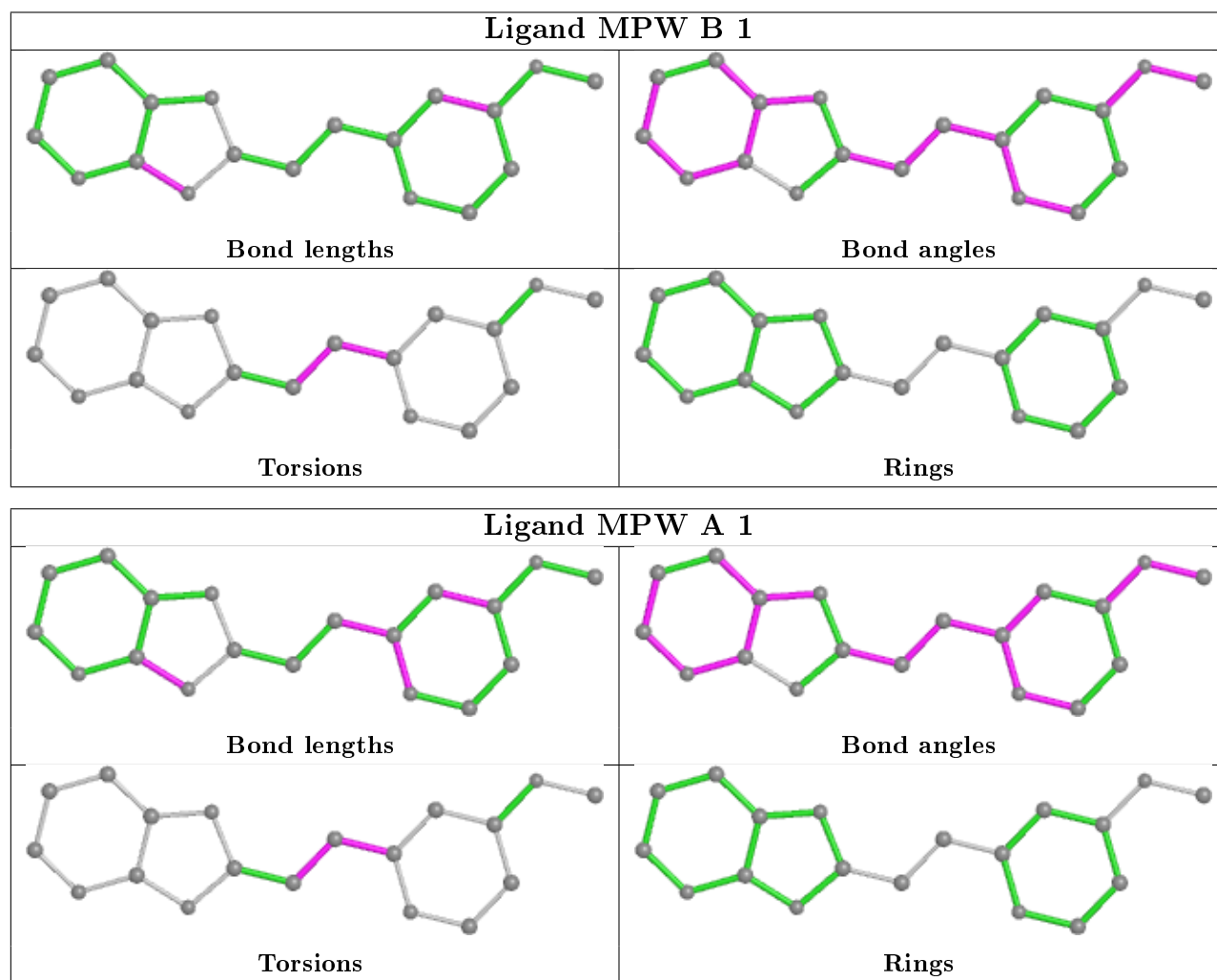
There are no ring outliers.

5 monomers are involved in 14 short contacts:

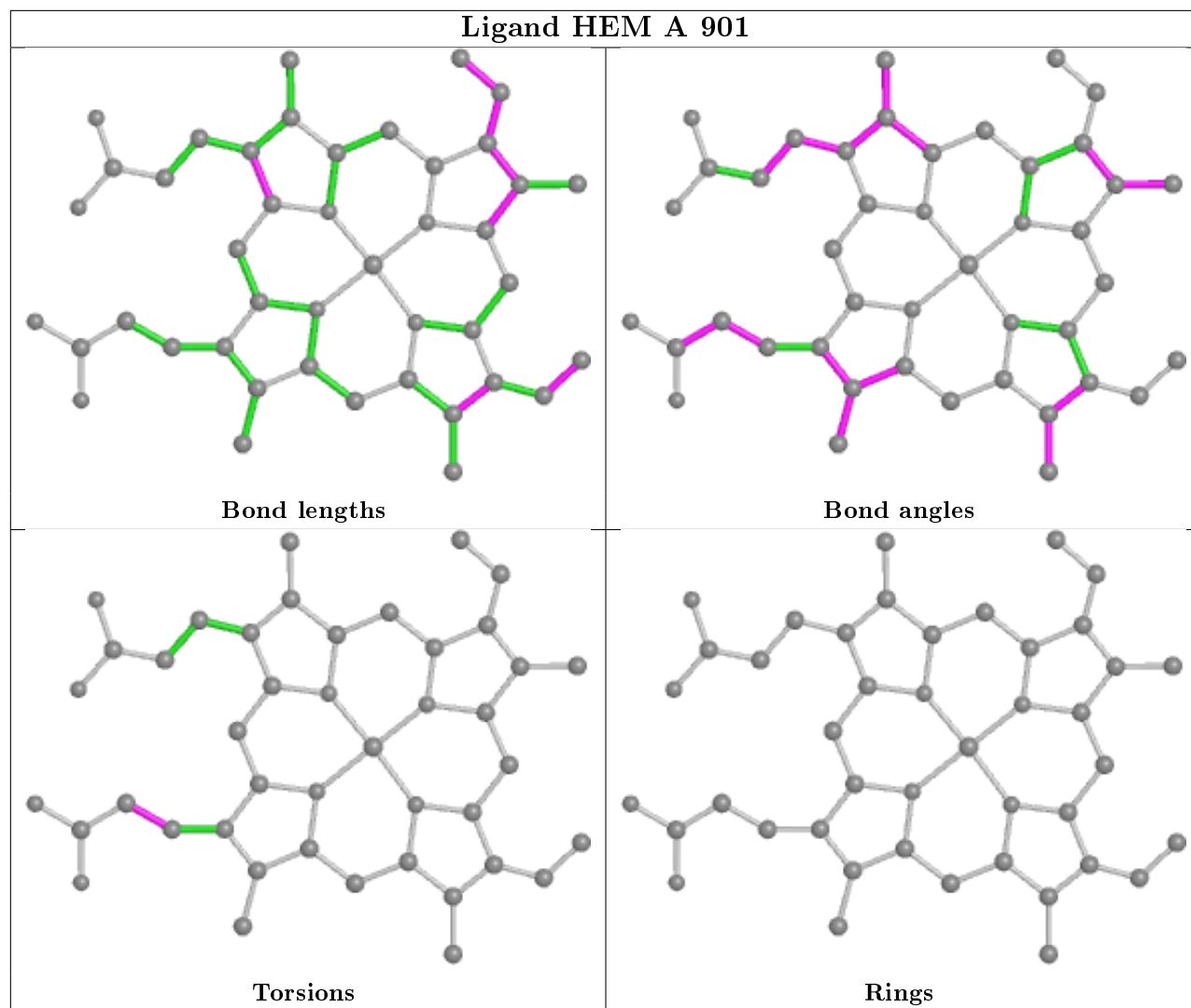
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1	MPW	3	0
5	A	1	MPW	2	0
3	A	902	H4B	1	0
2	A	901	HEM	6	0
2	B	901	HEM	3	0

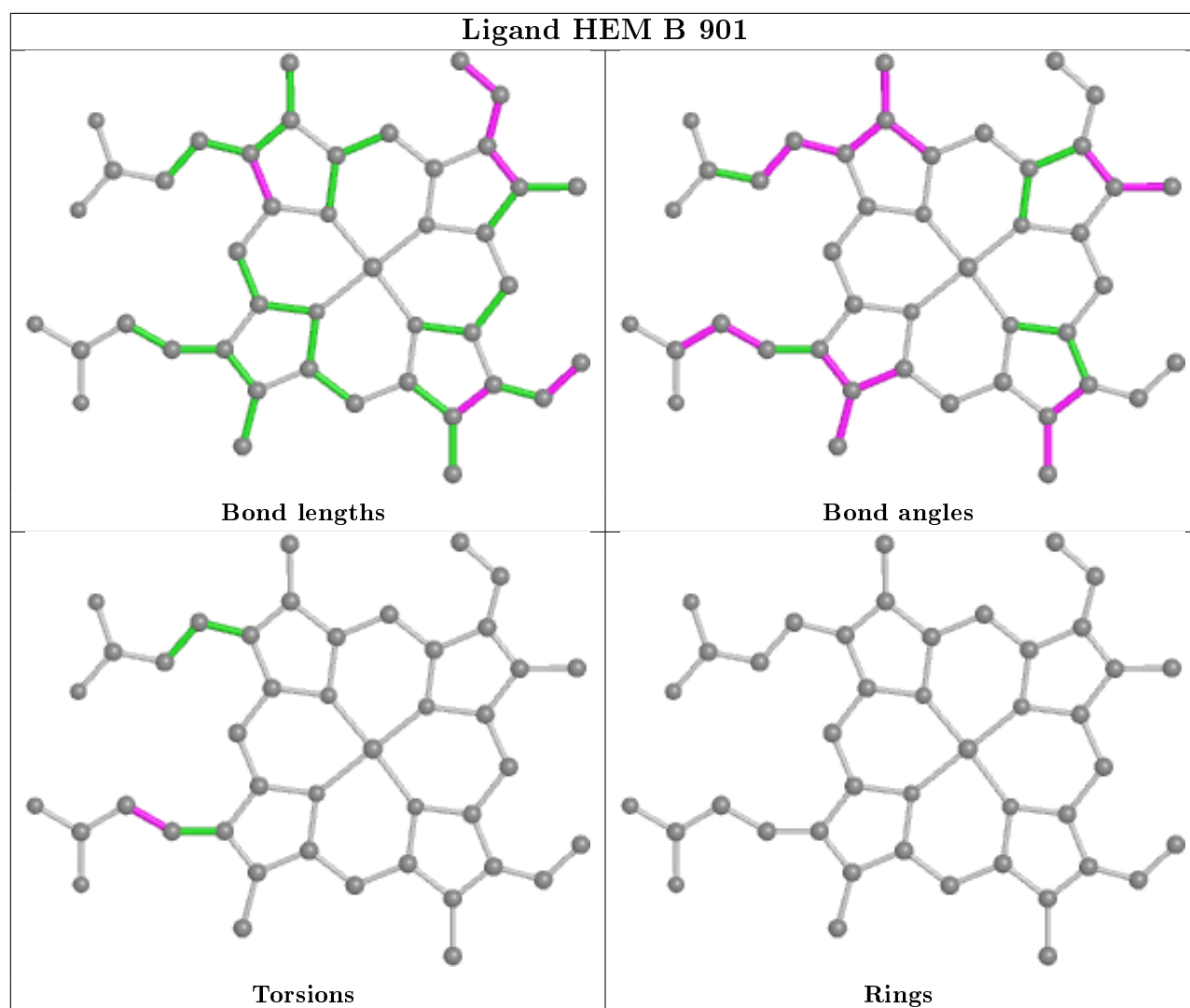
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	414/423 (97%)	0.07	23 (5%) 24 16	34, 74, 118, 155	0
1	B	413/423 (97%)	0.03	12 (2%) 51 41	33, 75, 118, 138	0
All	All	827/846 (97%)	0.05	35 (4%) 36 26	33, 75, 118, 155	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	108	SER	8.5
1	A	267	PRO	4.4
1	A	494	ILE	3.9
1	A	295	ARG	3.8
1	A	446	ARG	3.3
1	B	494	ILE	3.3
1	A	150	GLU	3.1
1	B	287	LEU	3.1
1	A	266	MET	3.0
1	B	150	GLU	3.0
1	B	394	GLY	2.8
1	A	100	SER	2.7
1	A	108	SER	2.7
1	B	446	ARG	2.7
1	A	85	GLY	2.7
1	A	290	LYS	2.7
1	A	109	CYS	2.7
1	B	148	PHE	2.6
1	A	270	THR	2.6
1	A	269	GLY	2.6
1	B	171	GLY	2.5
1	A	148	PHE	2.5
1	A	495	TRP	2.5
1	A	77	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	381	GLN	2.3
1	A	395	LEU	2.3
1	B	290	LYS	2.3
1	B	149	LYS	2.2
1	A	397	THR	2.2
1	A	396	GLU	2.1
1	A	491	LYS	2.1
1	A	152	LYS	2.1
1	B	267	PRO	2.1
1	A	383	TYR	2.0
1	B	154	GLU	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](#)

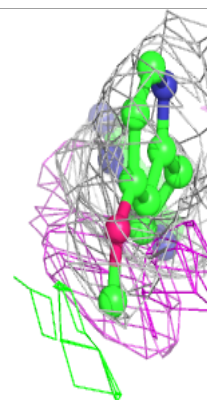
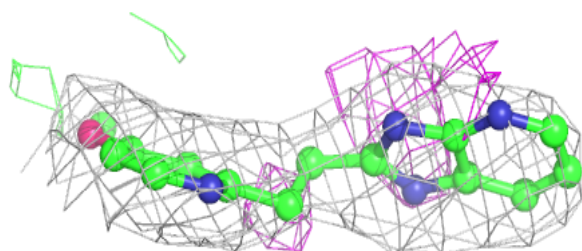
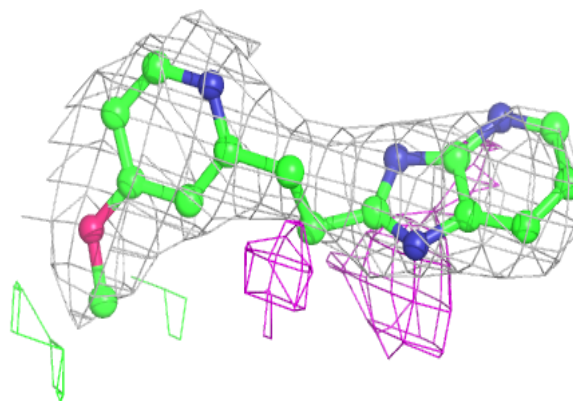
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
4	SO4	A	907	5/5	0.90	0.32	122,127,136,141	0
5	MPW	B	1	19/19	0.92	0.22	40,61,77,84	0
3	H4B	A	902	17/17	0.94	0.14	51,59,72,79	0
3	H4B	B	902	17/17	0.94	0.17	50,61,76,82	0
2	HEM	A	901	43/43	0.95	0.17	1,50,77,96	0
2	HEM	B	901	43/43	0.95	0.17	1,49,78,96	0
5	MPW	A	1	19/19	0.96	0.18	37,58,75,80	0

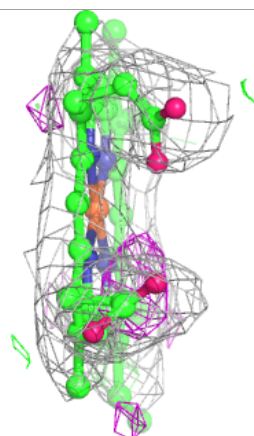
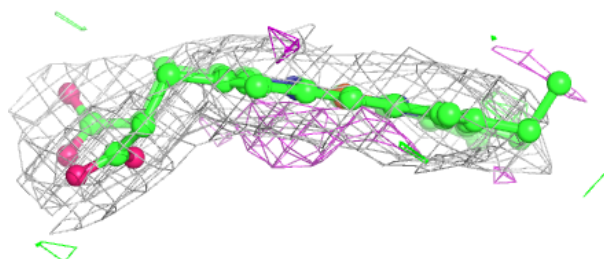
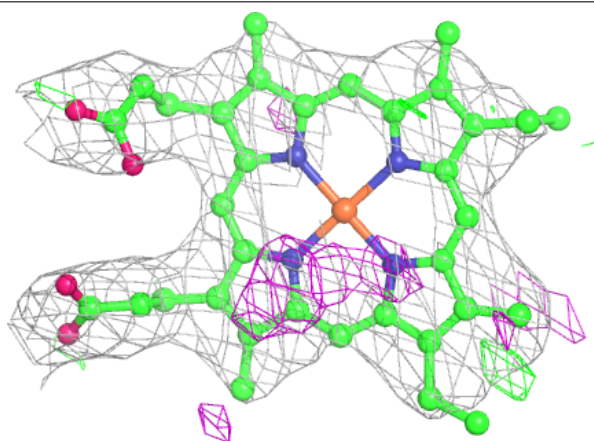
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around MPW B 1:**

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

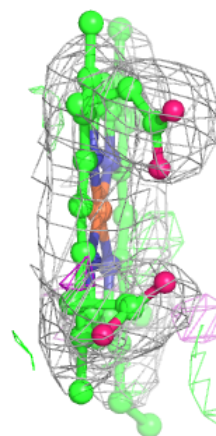
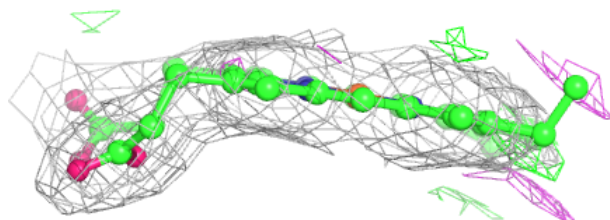
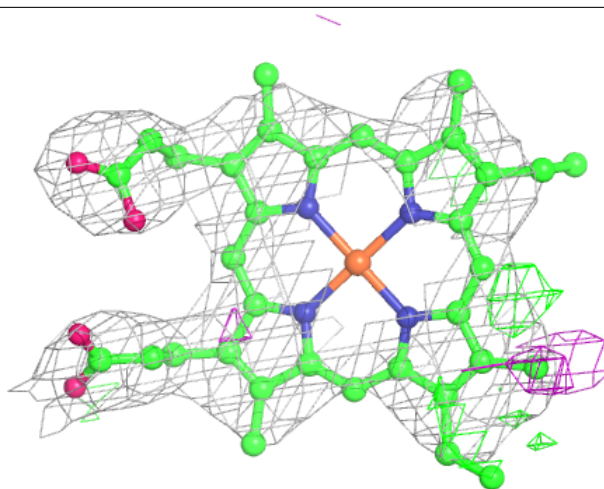
**Electron density around HEM A 901:**

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



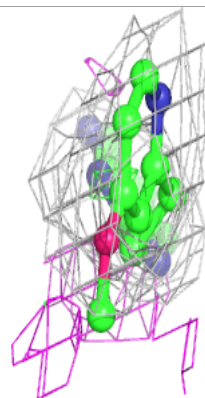
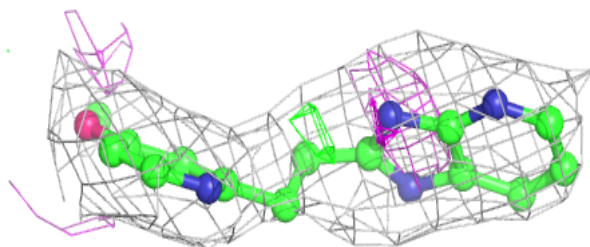
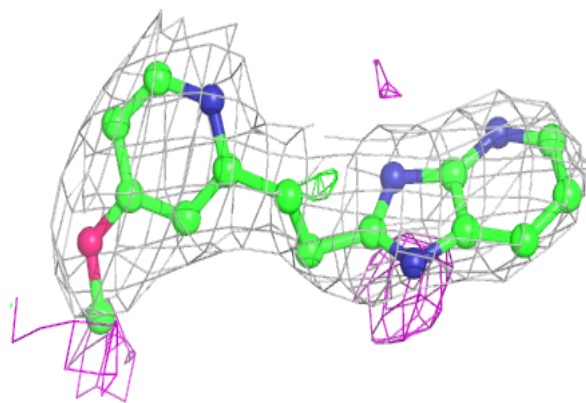
**Electron density around HEM B 901:**

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



**Electron density around MPW A 1:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.