



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 03:55 AM JST

PDB ID : 6KOC  
Title : X-ray Structure of the proton-pumping cytochrome aa3-600 menaquinol oxidase from *Bacillus subtilis* complexed with 3-iodo-N-oxo-2-heptyl-4-hydroxyquinoline  
Authors : Xu, J.; Ding, Z.; Liu, B.; Li, J.; Gennis, R.B.; Zhu, J.  
Deposited on : 2019-08-09  
Resolution : 3.80 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.

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

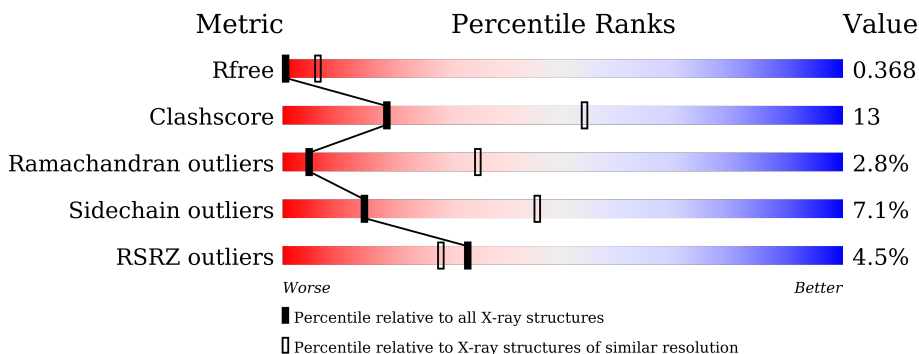
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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	649	 3% 60% 31% • 6%
1	E	649	 3% 64% 27% • 6%
2	B	296	 6% 44% 33% 9% 14%
2	F	296	 5% 53% 29% 5% 14%
3	C	204	 3% 69% 17% • 13%

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Mol	Chain	Length	Quality of chain
3	G	204	
4	D	123	
4	H	123	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	HEA	A	1002	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 17912 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 AA3-600 quinol oxidase subunit I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	607	4855	3270	752	792	41	0	0	0
1	E	607	4855	3270	752	792	41	0	0	0

- Molecule 2 is a protein called Quinol oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	256	2073	1348	328	390	7	0	0	0
2	F	256	2073	1348	328	390	7	0	0	0

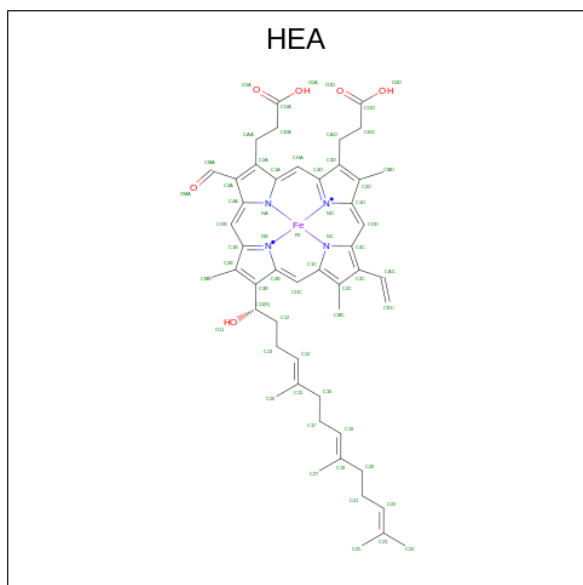
- Molecule 3 is a protein called AA3-600 quinol oxidase subunit IIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	178	1411	953	222	231	5	0	0	0
3	G	178	1411	953	222	231	5	0	0	0

- Molecule 4 is a protein called Quinol oxidase subunit 4, Quinol oxidase subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	70	482	317	78	84	3	0	0	0
4	H	70	482	317	78	84	3	0	0	0

- Molecule 5 is HEME-A (three-letter code: HEA) (formula:  $C_{49}H_{56}FeN_4O_6$ ).

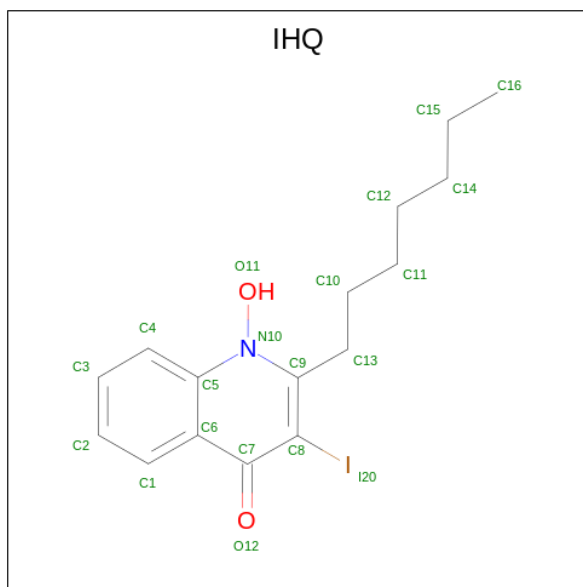


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	Fe	N			O	
5	A	1	Total	60	49	1	4	6	0	0
5	A	1	Total	60	49	1	4	6	0	0
5	E	1	Total	60	49	1	4	6	0	0
5	E	1	Total	60	49	1	4	6	0	0

- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
			Total	Cu			
6	A	1	Total	1	1	0	0
6	E	1	Total	1	1	0	0

- Molecule 7 is 2-heptyl-3-iodanyl-1-oxidanyl-quinolin-4-one (three-letter code: IHQ) (formula: C<sub>16</sub>H<sub>20</sub>INO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
7	A	1	Total	C	I	N	O	0	0
			14	10	1	1	2		
7	E	1	Total	C	I	N	O	0	0
			14	10	1	1	2		

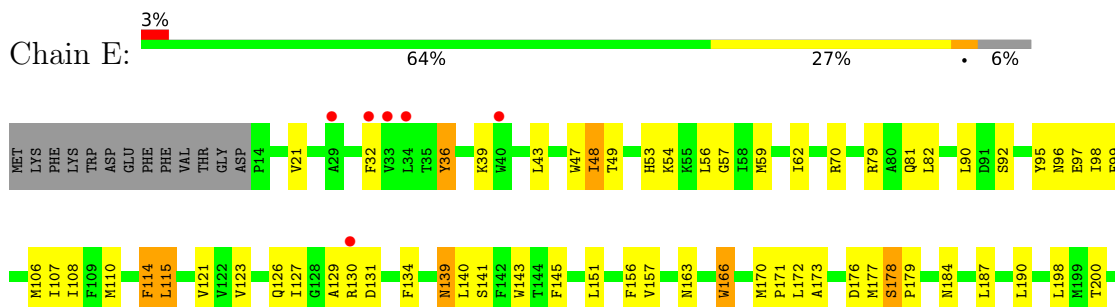
### 3 Residue-property plots [i](#)

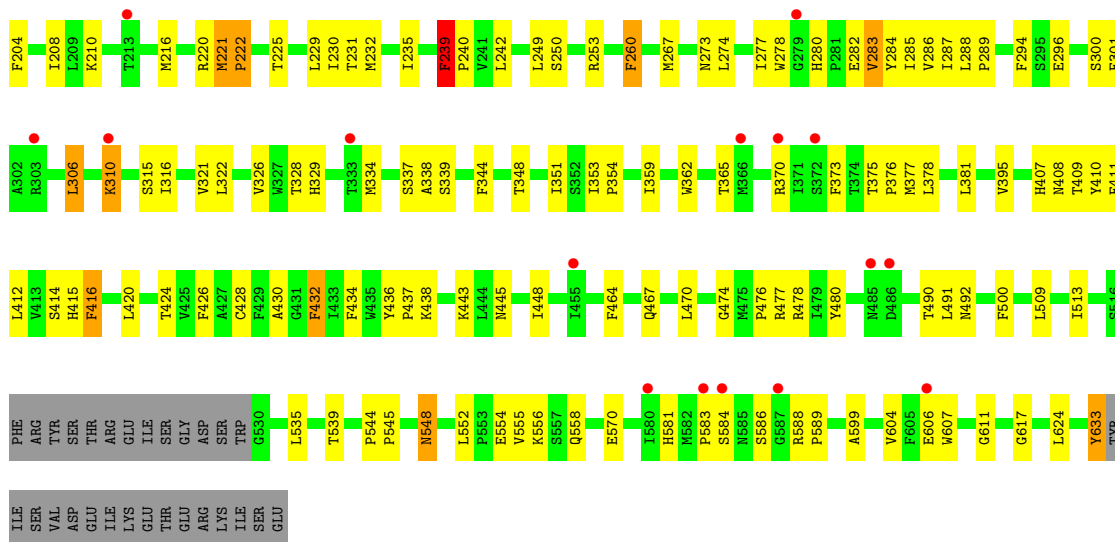
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: AA3-600 quinol oxidase subunit I

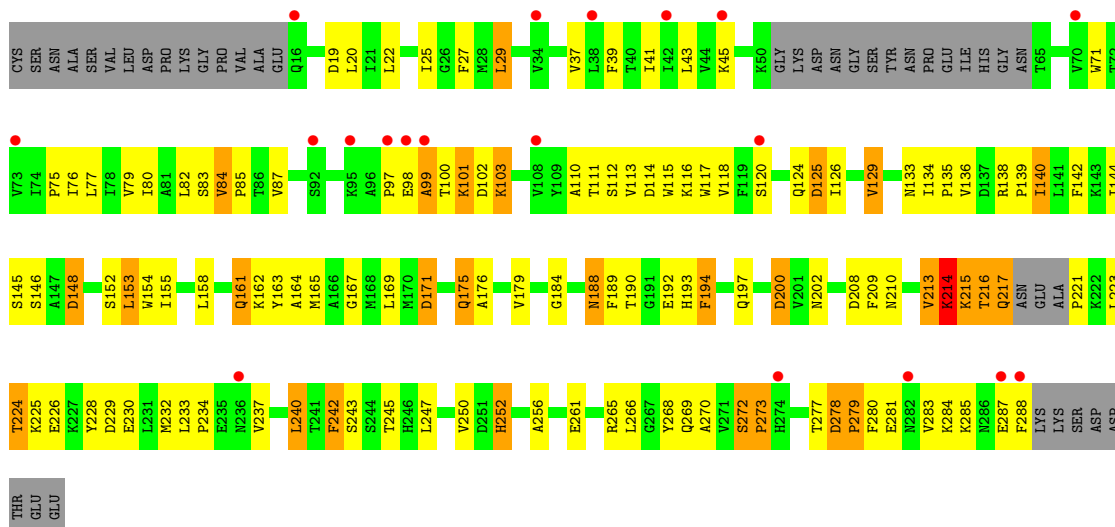


- Molecule 1: AA3-600 quinol oxidase subunit I

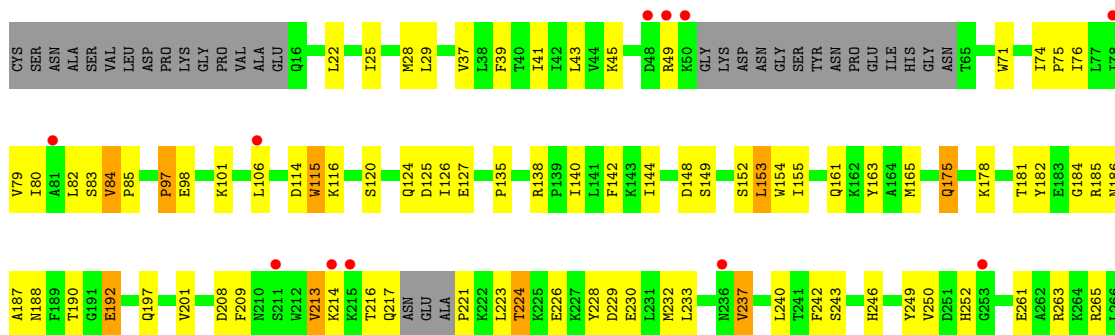




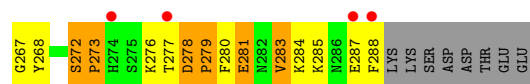
• Molecule 2: Quinol oxidase subunit 2



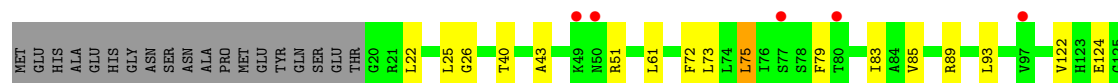
• Molecule 2: Quinol oxidase subunit 2







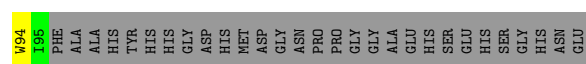
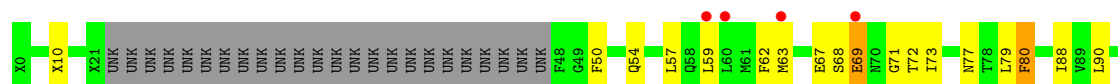
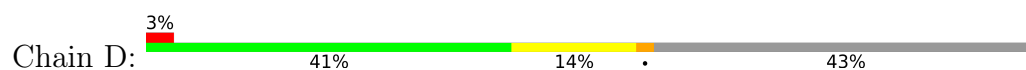
- Molecule 3: AA3-600 quinol oxidase subunit IIII



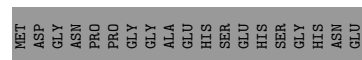
- Molecule 3: AA3-600 quinol oxidase subunit IIII



- Molecule 4: Quinol oxidase subunit 4, Quinol oxidase subunit 4



- Molecule 4: Quinol oxidase subunit 4, Quinol oxidase subunit 4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.93Å 162.20Å 151.32Å 90.00° 109.76° 90.00°	Depositor
Resolution (Å)	48.27 – 3.80 48.28 – 3.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.27-3.80) 98.0 (48.28-3.80)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 3.77Å)	Xtrriage
Refinement program	PHENIX 1.14_3235	Depositor
R, $R_{free}$	0.325 , 0.369 0.325 , 0.368	Depositor DCC
$R_{free}$ test set	2011 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	100.9	Xtrriage
Anisotropy	0.608	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.19 , 24.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.068 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.79	EDS
Total number of atoms	17912	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	128.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: IHQ, CU, HEA

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	0.26	0/5022	0.41	0/6827
1	E	0.25	0/5022	0.40	0/6827
2	B	0.30	0/2122	0.58	0/2879
2	F	0.26	0/2122	0.49	0/2879
3	C	0.24	0/1452	0.40	0/1974
3	G	0.24	0/1452	0.40	0/1974
4	D	0.26	0/381	0.40	0/514
4	H	0.26	0/381	0.41	0/514
All	All	0.26	0/17954	0.44	0/24388

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	214	LYS	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4855	0	4855	146	0
1	E	4855	0	4855	132	0
2	B	2073	0	2061	108	0
2	F	2073	0	2061	62	0
3	C	1411	0	1444	28	0
3	G	1411	0	1444	22	0
4	D	482	0	395	10	0
4	H	482	0	395	10	0
5	A	120	0	106	10	0
5	E	120	0	107	10	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
7	A	14	0	0	0	0
7	E	14	0	0	0	0
All	All	17912	0	17723	471	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 13.

All (471) 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)
2:B:148:ASP:OD1	2:B:148:ASP:N	2.03	0.92
1:A:332:PHE:O	2:B:162:LYS:NZ	2.03	0.91
2:B:214:LYS:HB2	2:B:217:GLN:H	1.38	0.89
1:E:170:MET:HG2	1:E:260:PHE:HB2	1.58	0.84
1:A:269:MET:HB3	2:B:165:MET:HE1	1.61	0.82
1:E:39:LYS:HE3	1:E:43:LEU:HB2	1.64	0.80
1:A:170:MET:HG2	1:A:260:PHE:HB2	1.65	0.79
2:F:214:LYS:HA	2:F:217:GLN:HE22	1.48	0.79
1:A:39:LYS:HE3	1:A:43:LEU:HB2	1.65	0.78
1:A:177:MET:HG2	1:A:179:PRO:HD2	1.66	0.76
2:B:217:GLN:HA	2:B:243:SER:HB2	1.68	0.75
1:E:177:MET:HG2	1:E:179:PRO:HD2	1.68	0.75
1:E:108:ILE:HG21	1:E:190:LEU:HD22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLY:H	2:B:162:LYS:HZ2	1.35	0.74
2:B:261:GLU:O	2:B:265:ARG:NH2	2.21	0.74
2:B:171:ASP:OD1	2:B:171:ASP:N	2.19	0.73
2:B:142:PHE:HB3	2:B:144:ILE:HD11	1.71	0.72
2:B:229:ASP:OD2	2:B:265:ARG:NH1	2.23	0.72
1:E:326:VAL:O	1:E:329:HIS:ND1	2.22	0.71
2:F:229:ASP:OD2	2:F:265:ARG:NH1	2.24	0.71
2:F:261:GLU:O	2:F:265:ARG:NH2	2.23	0.71
3:C:186:ASP:HA	3:C:189:TRP:HB2	1.73	0.70
1:A:108:ILE:HG21	1:A:190:LEU:HD22	1.73	0.70
1:E:409:THR:O	1:E:411:PHE:N	2.23	0.70
1:A:476:PRO:HG3	2:B:154:TRP:HZ3	1.57	0.70
1:E:409:THR:HA	1:E:476:PRO:HA	1.72	0.70
1:E:54:LYS:NZ	1:E:545:PRO:O	2.25	0.69
2:F:284:LYS:HD3	2:F:285:LYS:H	1.57	0.69
2:B:209:PHE:O	2:B:213:VAL:N	2.26	0.69
2:B:230:GLU:O	2:B:284:LYS:NZ	2.26	0.69
2:B:144:ILE:HG22	2:B:164:ALA:HB2	1.75	0.68
1:A:134:PHE:HZ	3:C:26:GLY:HA3	1.59	0.68
1:A:467:GLN:HA	1:A:470:LEU:HB2	1.76	0.68
1:A:54:LYS:NZ	1:A:545:PRO:O	2.26	0.67
3:C:85:VAL:HA	3:C:89:ARG:HB2	1.77	0.67
1:A:599:ALA:HB2	1:A:617:GLY:HA3	1.75	0.67
1:A:409:THR:HA	1:A:476:PRO:HA	1.76	0.67
2:B:221:PRO:O	2:B:243:SER:OG	2.11	0.66
1:A:267:MET:HG2	3:C:51:ARG:HE	1.60	0.65
2:B:155:ILE:HA	2:B:184:GLY:HA2	1.77	0.65
2:F:230:GLU:O	2:F:284:LYS:NZ	2.29	0.65
1:E:599:ALA:HB2	1:E:617:GLY:HA3	1.78	0.65
1:E:92:SER:O	1:E:96:ASN:ND2	2.28	0.65
2:B:136:VAL:HG11	2:B:179:VAL:HG22	1.79	0.65
1:A:187:LEU:HD21	1:A:249:LEU:HG	1.78	0.64
1:A:409:THR:O	1:A:411:PHE:N	2.24	0.64
2:F:148:ASP:OD2	2:F:263:ARG:NH2	2.30	0.64
1:A:92:SER:O	1:A:96:ASN:ND2	2.31	0.64
2:B:278:ASP:O	2:B:280:PHE:N	2.31	0.64
1:A:412:LEU:HD11	5:A:1002:HEA:HHA	1.80	0.63
1:E:187:LEU:HD21	1:E:249:LEU:HG	1.80	0.63
1:E:378:LEU:HD23	1:E:381:LEU:HD12	1.79	0.63
2:B:101:LYS:HG3	2:B:102:ASP:H	1.62	0.63
2:F:76:ILE:HA	2:F:79:VAL:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:LEU:O	1:E:492:ASN:ND2	2.31	0.63
1:E:286:VAL:O	1:E:424:THR:OG1	2.17	0.61
2:B:117:TRP:NE1	2:B:197:GLN:OE1	2.33	0.61
1:A:49:THR:OG1	1:A:586:SER:O	2.19	0.60
2:B:114:ASP:N	2:B:148:ASP:OD2	2.31	0.60
1:A:334:MET:HA	2:B:163:TYR:HB2	1.82	0.60
2:B:153:LEU:H	2:B:153:LEU:HD12	1.67	0.60
1:E:95:TYR:OH	5:E:1001:HEA:O1A	2.20	0.60
1:E:420:LEU:HD13	5:E:1002:HEA:HBC2	1.83	0.60
1:A:337:SER:O	1:A:339:SER:N	2.34	0.60
2:B:79:VAL:O	2:B:83:SER:N	2.35	0.60
2:F:37:VAL:HG13	2:F:41:ILE:HD12	1.84	0.60
1:A:204:PHE:HB2	1:A:232:MET:HG3	1.83	0.59
1:A:79:ARG:NH2	1:A:467:GLN:OE1	2.28	0.59
2:F:116:LYS:HD3	2:F:237:VAL:HG11	1.83	0.59
3:G:85:VAL:HA	3:G:89:ARG:HB2	1.85	0.59
1:A:53:HIS:HD2	1:A:131:ASP:HA	1.67	0.59
1:A:82:LEU:O	1:A:492:ASN:ND2	2.35	0.59
2:B:175:GLN:NE2	2:B:176:ALA:O	2.35	0.59
1:A:335:GLY:H	2:B:162:LYS:NZ	1.99	0.59
2:B:43:LEU:O	2:B:45:LYS:N	2.36	0.59
2:F:75:PRO:HB2	1:E:353:ILE:HD12	1.84	0.59
1:A:173:ALA:O	1:A:253:ARG:NH1	2.36	0.59
4:D:50:PHE:O	4:D:54:GLN:NE2	2.35	0.59
1:A:344:PHE:O	1:A:348:THR:OG1	2.19	0.59
2:B:269:GLN:NE2	2:F:281:GLU:OE2	2.35	0.58
1:E:220:ARG:HB3	1:E:558:GLN:HG3	1.83	0.58
1:E:467:GLN:HA	1:E:470:LEU:HB2	1.85	0.58
1:E:437:PRO:HG3	1:E:443:LYS:HB3	1.83	0.58
1:A:353:ILE:HD12	2:B:75:PRO:HB2	1.84	0.58
1:E:123:VAL:HG13	1:E:225:THR:HG23	1.85	0.58
1:A:470:LEU:HD11	1:A:492:ASN:HA	1.85	0.58
3:C:75:LEU:HD21	3:C:182:TRP:HE1	1.68	0.58
3:G:26:GLY:HA3	1:E:134:PHE:HZ	1.68	0.58
2:B:113:VAL:HA	2:B:148:ASP:OD1	2.04	0.58
1:E:315:SER:OG	1:E:354:PRO:O	2.21	0.58
4:D:71:GLY:O	4:D:73:ILE:N	2.38	0.57
2:F:98:GLU:O	2:F:175:GLN:NE2	2.34	0.57
1:A:123:VAL:HG13	1:A:225:THR:HG23	1.85	0.57
2:B:126:ILE:HD13	2:B:213:VAL:O	2.03	0.56
2:B:200:ASP:OD1	2:B:200:ASP:N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:THR:HB	2:B:139:PRO:HD3	1.87	0.56
3:C:190:ILE:HG21	4:D:57:LEU:HD13	1.87	0.56
1:A:378:LEU:HD23	1:A:381:LEU:HD12	1.87	0.56
1:A:414:SER:OG	1:A:464:PHE:O	2.18	0.56
2:B:233:LEU:HD11	2:B:266:LEU:HD12	1.87	0.56
2:F:84:VAL:H	2:F:85:PRO:HD2	1.71	0.56
2:F:221:PRO:O	2:F:243:SER:OG	2.20	0.56
1:A:554:GLU:HB3	1:A:556:LYS:HE3	1.88	0.56
2:B:175:GLN:HE21	2:B:176:ALA:C	2.09	0.56
2:B:76:ILE:HA	2:B:79:VAL:HG22	1.87	0.56
1:E:204:PHE:HB2	1:E:232:MET:HG3	1.88	0.56
2:B:114:ASP:HB3	2:B:234:PRO:HB3	1.86	0.56
2:B:84:VAL:H	2:B:85:PRO:HD2	1.71	0.55
3:C:122:VAL:HA	3:C:126:ALA:HB2	1.88	0.55
2:F:190:THR:HB	1:E:478:ARG:HB3	1.87	0.55
1:E:377:MET:O	1:E:381:LEU:N	2.38	0.55
3:C:141:LEU:HA	3:C:144:HIS:HB3	1.88	0.55
1:E:470:LEU:HD11	1:E:492:ASN:HA	1.87	0.55
1:A:286:VAL:O	1:A:424:THR:OG1	2.24	0.55
1:A:346:ILE:HD11	2:B:87:VAL:HG21	1.88	0.55
2:B:210:ASN:HA	2:B:213:VAL:HG12	1.88	0.55
1:E:445:ASN:HB3	1:E:448:ILE:HD11	1.88	0.55
1:E:554:GLU:HB3	1:E:556:LYS:HE3	1.89	0.55
3:C:83:ILE:HD13	3:C:176:PHE:HD1	1.72	0.54
2:F:209:PHE:O	2:F:213:VAL:HG13	2.08	0.54
1:A:134:PHE:CZ	3:C:26:GLY:HA3	2.40	0.54
1:A:54:LYS:HZ3	1:A:544:PRO:HB2	1.72	0.54
1:E:53:HIS:HD2	1:E:131:ASP:HA	1.72	0.54
1:E:414:SER:OG	1:E:464:PHE:O	2.21	0.54
1:A:53:HIS:CD2	1:A:131:ASP:HA	2.41	0.54
1:E:408:ASN:HB3	1:E:477:ARG:HG2	1.89	0.54
3:C:161:GLN:O	3:C:166:GLY:N	2.40	0.54
1:E:584:SER:HG	1:E:633:TYR:HH	1.54	0.54
1:A:79:ARG:HH22	1:A:495:SER:HB3	1.72	0.54
2:F:124:GLN:O	2:F:126:ILE:N	2.41	0.54
2:B:135:PRO:HG2	2:B:138:ARG:HD2	1.90	0.54
1:A:588:ARG:HE	1:A:624:LEU:HB3	1.73	0.53
2:B:163:TYR:CZ	2:B:189:PHE:HZ	2.27	0.53
1:E:49:THR:OG1	1:E:586:SER:O	2.24	0.53
1:E:230:ILE:HG13	1:E:316:ILE:HG23	1.89	0.53
3:C:194:THR:HG21	4:D:54:GLN:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:GLY:HA3	1:E:121:VAL:HG23	1.90	0.53
1:E:48:ILE:HA	1:E:143:TRP:HZ2	1.73	0.53
2:B:142:PHE:HD2	2:B:153:LEU:HD21	1.74	0.53
1:A:584:SER:OG	1:A:633:TYR:OH	2.23	0.53
1:E:337:SER:O	1:E:339:SER:N	2.41	0.53
2:B:240:LEU:HD12	2:B:242:PHE:HE1	1.74	0.53
1:E:21:VAL:HB	1:E:157:VAL:HG21	1.90	0.53
1:A:21:VAL:HB	1:A:157:VAL:HG21	1.91	0.53
2:B:37:VAL:HG13	2:B:41:ILE:HD12	1.90	0.53
4:H:88:ILE:HG12	1:E:277:ILE:HD13	1.90	0.53
1:A:412:LEU:HD13	5:A:1002:HEA:HBA1	1.91	0.52
2:B:100:THR:HB	2:B:139:PRO:HG3	1.91	0.52
1:E:53:HIS:CD2	1:E:131:ASP:HA	2.43	0.52
1:E:115:LEU:HG	1:E:289:PRO:HB2	1.89	0.52
3:G:40:THR:HG23	1:E:274:LEU:HD22	1.90	0.52
1:E:140:LEU:HB3	1:E:589:PRO:HB3	1.91	0.52
1:A:412:LEU:CD1	5:A:1002:HEA:HHA	2.39	0.52
1:A:184:ASN:HB3	1:A:604:VAL:HG22	1.92	0.52
4:H:71:GLY:O	4:H:73:ILE:N	2.40	0.52
1:A:123:VAL:HG21	1:A:228:THR:HG21	1.92	0.52
1:E:47:TRP:O	1:E:49:THR:N	2.43	0.52
1:A:476:PRO:HG3	2:B:154:TRP:CZ3	2.41	0.52
2:F:214:LYS:HA	2:F:217:GLN:NE2	2.21	0.52
2:B:99:ALA:HA	2:B:175:GLN:OE1	2.10	0.52
3:C:158:ILE:HD12	3:C:175:ILE:HG13	1.91	0.52
2:F:120:SER:HA	2:F:127:GLU:HA	1.91	0.52
2:F:213:VAL:O	2:F:217:GLN:NE2	2.43	0.52
1:A:408:ASN:HB3	1:A:477:ARG:HG2	1.92	0.51
1:E:373:PHE:CD1	1:E:381:LEU:HD11	2.45	0.51
1:A:54:LYS:NZ	1:A:544:PRO:HB2	2.25	0.51
3:G:186:ASP:HA	3:G:189:TRP:HB2	1.91	0.51
2:F:186:ASN:OD1	2:F:187:ALA:N	2.43	0.51
2:F:268:TYR:HD1	2:F:279:PRO:HD2	1.75	0.51
1:E:242:LEU:HB2	1:E:278:TRP:CG	2.46	0.51
1:A:126:GLN:HA	1:A:535:LEU:HB2	1.93	0.51
2:B:233:LEU:HB2	2:B:284:LYS:HZ1	1.76	0.51
1:E:301:PHE:HD2	1:E:377:MET:HG2	1.75	0.51
1:A:331:PHE:O	1:A:333:THR:N	2.38	0.51
1:A:115:LEU:HG	1:A:289:PRO:HB2	1.93	0.51
1:E:184:ASN:HB3	1:E:604:VAL:HG22	1.93	0.51
3:C:93:LEU:HD23	3:C:93:LEU:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:VAL:HB	2:B:29:LEU:HB3	1.92	0.50
1:E:54:LYS:NZ	1:E:544:PRO:HB2	2.27	0.50
2:B:224:THR:O	2:B:226:GLU:N	2.40	0.50
2:F:163:TYR:HB2	1:E:334:MET:HA	1.92	0.50
1:E:412:LEU:CD1	5:E:1002:HEA:HHA	2.42	0.50
3:G:26:GLY:HA3	1:E:134:PHE:CZ	2.47	0.50
1:E:588:ARG:HE	1:E:624:LEU:HB3	1.77	0.50
2:B:250:VAL:C	2:B:252:HIS:H	2.16	0.50
1:E:416:PHE:CZ	5:E:1001:HEA:HHD	2.47	0.50
2:B:99:ALA:HB2	2:B:175:GLN:HB2	1.93	0.49
1:E:106:MET:O	1:E:108:ILE:N	2.38	0.49
1:E:166:TRP:H	5:E:1001:HEA:CGD	2.25	0.49
3:C:188:VAL:HA	3:C:191:PHE:HB2	1.95	0.49
1:A:56:LEU:HD21	1:A:139:ASN:HA	1.95	0.49
1:A:57:GLY:HA3	1:A:121:VAL:HG23	1.94	0.49
1:A:141:SER:OG	1:A:200:THR:OG1	2.29	0.49
2:B:124:GLN:O	2:B:126:ILE:N	2.46	0.49
3:C:75:LEU:HD11	3:C:182:TRP:HE1	1.75	0.49
2:F:71:TRP:O	2:F:75:PRO:HD3	2.12	0.49
1:E:280:HIS:HA	1:E:283:VAL:HB	1.95	0.49
3:G:93:LEU:HD23	3:G:93:LEU:H	1.77	0.49
1:A:242:LEU:HB2	1:A:278:TRP:CD1	2.47	0.49
2:B:80:ILE:HD12	2:B:83:SER:HB3	1.95	0.49
1:E:428:CYS:O	1:E:432:PHE:HB2	2.13	0.49
1:A:284:TYR:HA	1:A:287:ILE:HG22	1.94	0.49
3:C:22:LEU:HD23	3:C:22:LEU:H	1.77	0.49
1:E:296:GLU:O	1:E:300:SER:N	2.45	0.49
1:E:326:VAL:HG22	1:E:329:HIS:HD1	1.78	0.49
2:B:250:VAL:O	2:B:252:HIS:N	2.43	0.49
2:F:182:TYR:HB2	2:F:201:VAL:HG23	1.95	0.49
1:E:306:LEU:HD23	1:E:365:THR:HG21	1.93	0.49
1:E:359:ILE:HA	1:E:362:TRP:CE3	2.47	0.49
1:A:445:ASN:HB3	1:A:448:ILE:HD11	1.94	0.49
2:B:284:LYS:HD3	2:B:285:LYS:H	1.77	0.49
2:F:278:ASP:O	2:F:280:PHE:N	2.45	0.49
1:E:208:ILE:HD13	1:E:229:LEU:HB2	1.95	0.49
1:E:284:TYR:HA	1:E:287:ILE:HG22	1.94	0.48
3:G:194:THR:HG21	4:H:54:GLN:HG3	1.94	0.48
1:E:412:LEU:HD11	5:E:1002:HEA:HHA	1.94	0.48
1:A:274:LEU:HD22	3:C:40:THR:HG23	1.95	0.48
1:A:437:PRO:HG3	1:A:443:LYS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:LYS:NZ	1:E:548:ASN:HB3	2.28	0.48
1:A:47:TRP:O	1:A:49:THR:N	2.46	0.48
1:A:187:LEU:HD23	1:A:250:SER:HA	1.96	0.48
2:B:188:ASN:HD22	2:B:188:ASN:C	2.17	0.48
1:E:187:LEU:HD23	1:E:250:SER:HA	1.96	0.48
2:B:114:ASP:O	2:B:116:LYS:N	2.44	0.48
2:F:268:TYR:CD1	2:F:279:PRO:HD2	2.49	0.48
1:A:220:ARG:HB3	1:A:558:GLN:HG3	1.96	0.48
1:A:420:LEU:HD23	5:A:1001:HEA:HAC	1.95	0.48
2:B:158:LEU:HD22	2:B:175:GLN:O	2.14	0.48
1:A:95:TYR:OH	5:A:1001:HEA:O1A	2.30	0.48
1:A:246:LEU:O	1:A:250:SER:N	2.39	0.48
1:A:178:SER:HB2	2:B:270:ALA:O	2.13	0.48
1:E:126:GLN:HA	1:E:535:LEU:HB2	1.95	0.48
2:B:233:LEU:HB2	2:B:284:LYS:NZ	2.28	0.48
1:E:426:PHE:O	1:E:430:ALA:N	2.40	0.48
1:E:607:TRP:HD1	1:E:611:GLY:HA2	1.79	0.48
1:A:90:LEU:HD13	1:A:98:ILE:HD12	1.96	0.47
1:A:103:GLY:HA3	5:A:1001:HEA:HBD2	1.96	0.47
1:E:121:VAL:HG13	1:E:438:LYS:NZ	2.29	0.47
1:A:96:ASN:OD1	2:B:190:THR:OG1	2.26	0.47
1:A:584:SER:HG	1:A:633:TYR:HH	1.46	0.47
1:E:242:LEU:HB2	1:E:278:TRP:CD1	2.49	0.47
2:F:155:ILE:HA	2:F:184:GLY:HA2	1.96	0.47
3:C:75:LEU:HD11	3:C:182:TRP:NE1	2.30	0.47
3:G:28:TRP:HZ2	4:H:66:THR:HG22	1.80	0.47
3:G:75:LEU:HD21	3:G:182:TRP:HE1	1.79	0.47
1:E:56:LEU:HD21	1:E:139:ASN:HA	1.96	0.47
1:A:110:MET:O	1:A:114:PHE:HB2	2.15	0.47
1:A:206:VAL:HG21	3:C:26:GLY:HA2	1.97	0.47
3:G:153:PHE:HA	3:G:156:THR:HG22	1.96	0.47
2:F:49:ARG:HG2	1:E:370:ARG:NE	2.31	0.47
1:E:280:HIS:CG	1:E:329:HIS:HE1	2.33	0.47
1:A:280:HIS:HA	1:A:283:VAL:HB	1.97	0.46
1:A:376:PRO:HG3	1:A:433:ILE:HG22	1.98	0.46
2:B:133:ASN:HA	2:B:202:ASN:O	2.16	0.46
2:B:215:LYS:HA	2:B:215:LYS:HD2	1.66	0.46
2:F:43:LEU:O	2:F:45:LYS:N	2.46	0.46
1:E:322:LEU:HB3	1:E:351:ILE:HD12	1.96	0.46
1:A:180:GLY:O	1:A:253:ARG:NH2	2.47	0.46
1:A:533:ARG:NH1	1:A:559:ASP:OD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:141:LEU:HA	3:G:144:HIS:HB3	1.97	0.46
4:H:68:SER:O	4:H:70:ASN:N	2.49	0.46
1:A:235:ILE:O	1:A:239:PHE:HB2	2.16	0.46
2:B:140:ILE:HB	2:B:142:PHE:HE1	1.80	0.46
2:B:245:THR:HG22	2:B:247:LEU:H	1.80	0.46
2:F:267:GLY:HA3	2:F:281:GLU:HG3	1.97	0.46
2:F:276:LYS:HE2	2:F:277:THR:H	1.81	0.46
1:E:96:ASN:HB3	1:E:163:ASN:HB2	1.97	0.46
1:A:322:LEU:HB3	1:A:351:ILE:HD12	1.98	0.46
1:A:353:ILE:HB	1:A:354:PRO:HD3	1.97	0.46
3:G:193:PHE:HA	3:G:197:TYR:HD2	1.80	0.46
1:A:54:LYS:NZ	1:A:548:ASN:HB3	2.31	0.46
1:A:178:SER:OG	1:A:179:PRO:HD3	2.15	0.46
1:E:235:ILE:O	1:E:239:PHE:HB2	2.16	0.46
1:E:607:TRP:CD1	1:E:611:GLY:HA2	2.51	0.46
1:A:106:MET:O	1:A:108:ILE:N	2.42	0.46
1:E:198:LEU:HD11	1:E:240:PRO:HG3	1.98	0.46
2:B:100:THR:OG1	2:B:103:LYS:O	2.33	0.46
2:B:101:LYS:CG	2:B:102:ASP:H	2.29	0.46
2:F:135:PRO:HG2	2:F:138:ARG:HD2	1.98	0.46
1:E:353:ILE:HB	1:E:354:PRO:HD3	1.98	0.46
1:E:106:MET:HA	1:E:110:MET:HB3	1.98	0.45
1:A:393:THR:HG21	1:A:468:TYR:CZ	2.50	0.45
2:B:142:PHE:HB3	2:B:144:ILE:CD1	2.43	0.45
2:B:112:SER:H	2:B:146:SER:HA	1.81	0.45
2:B:230:GLU:OE1	2:B:285:LYS:NZ	2.45	0.45
2:F:106:LEU:HD22	2:F:138:ARG:HH21	1.81	0.45
1:E:32:PHE:HA	1:E:36:TYR:HB2	1.99	0.45
1:E:39:LYS:HA	1:E:39:LYS:HD2	1.82	0.45
1:E:376:PRO:HB3	1:E:434:PHE:HB2	1.98	0.45
2:B:111:THR:HG21	2:B:252:HIS:CD2	2.51	0.45
2:F:250:VAL:C	2:F:252:HIS:H	2.20	0.45
1:A:329:HIS:C	1:A:329:HIS:CD2	2.90	0.45
1:A:420:LEU:HD13	5:A:1002:HEA:HBC2	1.98	0.45
2:B:110:ALA:HB3	2:B:144:ILE:HD13	1.99	0.45
1:E:412:LEU:HD11	5:E:1002:HEA:HAD2	1.99	0.45
1:A:416:PHE:CZ	5:A:1001:HEA:HHD	2.51	0.45
2:B:100:THR:HG23	2:B:101:LYS:O	2.17	0.45
2:F:120:SER:HB3	2:F:127:GLU:HG3	1.99	0.45
2:F:224:THR:O	2:F:226:GLU:N	2.42	0.45
1:E:81:GLN:NE2	1:E:480:TYR:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:ILE:HG12	1:E:285:ILE:HD13	1.98	0.45
3:G:28:TRP:CZ2	4:H:66:THR:HG22	2.52	0.45
2:F:217:GLN:OE1	2:F:217:GLN:N	2.50	0.45
3:G:155:ILE:O	3:G:159:LEU:HD23	2.18	0.44
1:E:344:PHE:O	1:E:348:THR:OG1	2.25	0.44
3:C:73:LEU:HD23	4:D:10:UNK:HA	1.98	0.44
2:B:214:LYS:HB3	2:B:217:GLN:NE2	2.33	0.44
2:F:140:ILE:HD12	2:F:142:PHE:CZ	2.52	0.44
1:E:121:VAL:HG13	1:E:438:LYS:HZ2	1.83	0.44
1:A:54:LYS:HZ1	1:A:548:ASN:HB3	1.83	0.44
1:A:121:VAL:HG13	1:A:438:LYS:HZ2	1.83	0.44
1:A:490:THR:HG23	1:A:491:LEU:HD22	2.00	0.44
3:C:188:VAL:HG23	3:C:189:TRP:HE3	1.83	0.44
4:H:59:LEU:O	4:H:63:MET:HB2	2.17	0.44
3:G:51:ARG:HE	1:E:267:MET:HG2	1.82	0.44
3:G:104:LEU:HD11	3:G:152:ILE:HG23	1.98	0.44
2:F:142:PHE:HB3	2:F:144:ILE:HD11	1.99	0.44
1:E:36:TYR:HA	1:E:39:LYS:HG2	2.00	0.44
1:A:106:MET:HB3	1:A:107:ILE:HD12	1.99	0.44
1:A:136:TYR:OH	1:A:588:ARG:HD3	2.17	0.44
1:A:198:LEU:HD11	1:A:240:PRO:HG3	2.00	0.44
1:A:319:ILE:HG23	1:A:354:PRO:HB2	2.00	0.44
1:E:231:THR:HG23	1:E:285:ILE:HG23	1.99	0.44
1:A:244:VAL:HA	1:A:247:ALA:HB3	1.99	0.44
2:B:114:ASP:C	2:B:116:LYS:H	2.20	0.44
3:G:86:HIS:CD2	3:G:92:SER:HB2	2.52	0.44
2:F:154:TRP:HZ3	1:E:476:PRO:HG3	1.82	0.44
2:F:185:ARG:HD3	1:E:476:PRO:HG2	2.00	0.44
1:E:178:SER:OG	1:E:179:PRO:HD3	2.18	0.44
1:A:72:GLY:HA2	5:A:1001:HEA:H14	2.00	0.43
2:F:115:TRP:HA	2:F:197:GLN:NE2	2.33	0.43
2:F:152:SER:OG	2:F:187:ALA:HB2	2.17	0.43
2:F:163:TYR:OH	1:E:407:HIS:NE2	2.46	0.43
1:E:90:LEU:HD13	1:E:98:ILE:HD12	1.99	0.43
1:E:509:LEU:O	1:E:513:ILE:HG13	2.18	0.43
1:A:96:ASN:HB3	1:A:163:ASN:HB2	2.00	0.43
1:A:106:MET:HA	1:A:110:MET:HB3	2.00	0.43
1:A:107:ILE:HA	1:A:111:ALA:HB3	1.98	0.43
2:B:145:SER:C	2:B:164:ALA:HB1	2.38	0.43
2:B:272:SER:OG	2:B:273:PRO:HD3	2.18	0.43
1:E:79:ARG:NH2	1:E:467:GLN:OE1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:TYR:O	1:A:414:SER:N	2.38	0.43
2:B:135:PRO:CG	2:B:138:ARG:HD2	2.48	0.43
2:B:154:TRP:HA	2:B:161:GLN:HB3	2.00	0.43
2:B:154:TRP:HA	2:B:161:GLN:CB	2.49	0.43
4:H:67:GLU:HA	4:H:68:SER:HA	1.65	0.43
1:A:397:LEU:HD12	5:A:1002:HEA:HBA2	2.00	0.43
3:G:87:GLU:HB3	3:G:169:PRO:HB3	2.00	0.43
1:E:127:ILE:HG13	1:E:129:ALA:H	1.84	0.43
2:B:117:TRP:CZ3	2:B:153:LEU:HB3	2.54	0.43
1:E:173:ALA:O	1:E:253:ARG:NH1	2.51	0.43
2:B:100:THR:HB	2:B:139:PRO:CG	2.49	0.43
2:B:268:TYR:HD1	2:B:279:PRO:HD2	1.82	0.43
3:C:167:LEU:HD13	3:C:171:THR:HG22	2.00	0.43
1:E:490:THR:HG23	1:E:491:LEU:HD22	2.01	0.43
1:A:607:TRP:HD1	1:A:611:GLY:HA2	1.83	0.43
2:B:111:THR:HA	2:B:145:SER:O	2.18	0.43
1:E:221:MET:N	1:E:222:PRO:HA	2.33	0.43
1:E:416:PHE:CD1	5:E:1002:HEA:HMD3	2.54	0.43
1:E:539:THR:HG21	1:E:544:PRO:HG3	2.00	0.43
2:B:80:ILE:HA	2:B:83:SER:HB3	2.01	0.43
2:B:140:ILE:HB	2:B:142:PHE:CE1	2.53	0.43
3:C:144:HIS:CE1	3:C:189:TRP:CE2	3.06	0.43
2:F:272:SER:OG	2:F:273:PRO:HD3	2.18	0.43
1:A:48:ILE:HA	1:A:143:TRP:HZ2	1.83	0.43
2:F:233:LEU:HB2	2:F:284:LYS:NZ	2.34	0.43
1:A:140:LEU:HB3	1:A:589:PRO:HB3	2.01	0.42
1:A:187:LEU:HD11	1:A:249:LEU:HD23	2.01	0.42
1:A:120:ASN:HA	1:A:204:PHE:HZ	1.83	0.42
1:A:230:ILE:HG13	1:A:316:ILE:HG23	2.00	0.42
1:A:406:TYR:HE2	2:B:22:LEU:HD22	1.83	0.42
2:F:228:TYR:HD2	2:F:249:TYR:HD2	1.67	0.42
1:E:106:MET:HB3	1:E:107:ILE:HD12	2.01	0.42
1:A:127:ILE:HG13	1:A:129:ALA:H	1.84	0.42
1:E:588:ARG:NE	1:E:624:LEU:HB3	2.34	0.42
1:A:185:TYR:CG	1:A:604:VAL:HG11	2.55	0.42
2:F:79:VAL:O	2:F:83:SER:N	2.47	0.42
2:F:97:PRO:HB2	2:F:98:GLU:H	1.59	0.42
2:F:154:TRP:CZ3	1:E:476:PRO:HG3	2.54	0.42
1:A:231:THR:HG23	1:A:285:ILE:HG23	2.00	0.42
1:A:331:PHE:C	1:A:333:THR:H	2.19	0.42
2:B:167:GLY:N	2:B:256:ALA:HB2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:MET:HA	1:E:62:ILE:HG22	2.00	0.42
1:A:221:MET:N	1:A:222:PRO:HA	2.34	0.42
1:A:396:MET:O	1:A:406:TYR:OH	2.25	0.42
1:A:551:VAL:HG22	1:A:572:TYR:HD1	1.84	0.42
1:A:588:ARG:NE	1:A:624:LEU:HB3	2.33	0.42
2:B:152:SER:HB3	2:B:163:TYR:HA	2.00	0.42
2:B:223:LEU:HD13	2:B:225:LYS:H	1.83	0.42
2:B:19:ASP:HA	2:B:22:LEU:HG	2.02	0.42
2:B:100:THR:HB	2:B:139:PRO:CD	2.50	0.42
1:E:282:GLU:HA	1:E:285:ILE:HD12	2.00	0.42
1:A:67:MET:HB3	1:A:105:ILE:HG23	2.01	0.42
2:B:77:LEU:HA	2:B:80:ILE:HG22	2.02	0.42
2:B:194:PHE:CE1	2:B:197:GLN:NE2	2.87	0.42
3:C:153:PHE:HA	3:C:156:THR:HG22	2.01	0.42
1:A:428:CYS:O	1:A:432:PHE:HB2	2.20	0.42
2:F:114:ASP:O	2:F:116:LYS:N	2.47	0.42
1:A:547:TYR:HA	1:A:581:HIS:HE2	1.85	0.42
3:C:158:ILE:HD12	3:C:175:ILE:HA	2.02	0.42
1:A:240:PRO:O	1:A:244:VAL:HG22	2.20	0.41
1:A:282:GLU:HA	1:A:285:ILE:HD12	2.02	0.41
3:C:43:ALA:HB2	4:D:88:ILE:HG22	2.01	0.41
1:A:235:ILE:HG12	1:A:285:ILE:HD13	2.01	0.41
2:F:25:ILE:HD11	2:F:82:LEU:HG	2.02	0.41
1:A:304:LYS:HG2	1:A:305:GLN:H	1.85	0.41
3:G:90:ARG:HH11	3:G:90:ARG:HA	1.84	0.41
2:F:178:LYS:O	2:F:182:TYR:OH	2.24	0.41
1:E:82:LEU:HD21	1:E:480:TYR:HA	2.02	0.41
1:E:114:PHE:HB3	1:E:428:CYS:SG	2.60	0.41
1:E:235:ILE:CG1	1:E:285:ILE:HD13	2.50	0.41
1:A:280:HIS:CE1	1:A:329:HIS:HE1	2.37	0.41
1:A:335:GLY:N	2:B:162:LYS:HZ2	2.11	0.41
1:A:349:MET:HB3	2:B:79:VAL:HB	2.03	0.41
1:A:426:PHE:O	1:A:430:ALA:N	2.49	0.41
2:B:25:ILE:HD12	2:B:25:ILE:HA	1.86	0.41
2:B:82:LEU:HD13	2:B:82:LEU:HA	1.90	0.41
4:D:77:ASN:HA	4:D:80:PHE:CE1	2.55	0.41
3:G:21:ARG:HA	3:G:21:ARG:HD3	1.84	0.41
3:G:24:ILE:O	3:G:28:TRP:HB2	2.20	0.41
4:H:80:PHE:HE1	1:E:321:VAL:HG23	1.86	0.41
1:E:294:PHE:HZ	1:E:426:PHE:HB3	1.86	0.41
1:E:416:PHE:CE2	5:E:1001:HEA:HHD	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:588:ARG:NE	1:E:624:LEU:O	2.51	0.41
1:A:170:MET:N	1:A:171:PRO:HD2	2.35	0.41
1:A:303:ARG:HG2	1:A:531:VAL:HG11	2.02	0.41
1:A:347:THR:O	1:A:351:ILE:HG12	2.20	0.41
1:A:418:TYR:HA	1:A:460:PHE:HZ	1.86	0.41
1:E:54:LYS:HG2	1:E:438:LYS:HZ1	1.85	0.41
1:E:170:MET:N	1:E:171:PRO:HD2	2.36	0.41
1:A:586:SER:O	1:A:589:PRO:HD2	2.20	0.41
2:B:287:GLU:HG2	2:B:288:PHE:H	1.85	0.41
2:F:80:ILE:HD12	2:F:80:ILE:HA	1.96	0.41
2:F:192:GLU:HA	1:E:92:SER:HB3	2.02	0.41
1:E:375:THR:HB	1:E:376:PRO:HD3	2.03	0.41
1:E:606:GLU:HB3	1:E:607:TRP:CE3	2.55	0.41
1:A:133:ALA:N	1:A:207:THR:OG1	2.51	0.41
1:A:212:ARG:HH12	1:A:218:LEU:HD12	1.85	0.41
2:B:117:TRP:O	2:B:129:VAL:HG22	2.21	0.41
4:D:90:LEU:O	4:D:94:TRP:HB2	2.21	0.41
2:F:149:SER:HB3	1:E:176:ASP:OD2	2.21	0.41
2:F:154:TRP:HA	2:F:161:GLN:HB3	2.03	0.41
2:F:250:VAL:O	2:F:252:HIS:N	2.49	0.41
1:E:141:SER:OG	1:E:200:THR:OG1	2.37	0.41
1:E:420:LEU:HD13	5:E:1002:HEA:CBC	2.49	0.41
1:A:39:LYS:HA	1:A:39:LYS:HD2	1.86	0.41
1:A:357:VAL:HG12	2:B:71:TRP:CZ3	2.56	0.41
2:F:74:ILE:N	2:F:75:PRO:CD	2.84	0.41
2:F:144:ILE:HD12	2:F:153:LEU:HD11	2.03	0.41
1:E:54:LYS:HZ1	1:E:548:ASN:HB3	1.86	0.41
1:E:97:GLU:HG2	1:E:163:ASN:HB3	2.02	0.41
2:B:111:THR:HB	2:B:118:VAL:HB	2.03	0.40
4:D:59:LEU:O	4:D:63:MET:HB2	2.20	0.40
1:E:586:SER:O	1:E:589:PRO:HD2	2.21	0.40
1:A:41:LYS:HD2	1:A:41:LYS:HA	1.88	0.40
2:B:214:LYS:HD2	2:B:216:THR:HA	2.03	0.40
4:H:70:ASN:OD1	1:E:210:LYS:NZ	2.53	0.40
2:F:287:GLU:HG2	2:F:288:PHE:H	1.86	0.40
1:E:310:LYS:H	1:E:310:LYS:HG3	1.69	0.40
2:B:124:GLN:CD	2:B:217:GLN:HE21	2.25	0.40
4:D:67:GLU:HA	4:D:68:SER:HA	1.66	0.40
1:A:62:ILE:HD12	1:A:62:ILE:HA	1.97	0.40
1:A:97:GLU:HG2	1:A:163:ASN:HB3	2.03	0.40
1:A:242:LEU:HB2	1:A:278:TRP:CG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:GLU:O	1:A:450:LYS:HD3	2.21	0.40
2:B:120:SER:HB2	2:B:245:THR:HG23	2.04	0.40
3:C:155:ILE:O	3:C:158:ILE:HG12	2.21	0.40
1:A:185:TYR:CD1	1:A:604:VAL:HG11	2.56	0.40
1:A:248:LEU:HD22	1:A:259:PHE:CZ	2.56	0.40
1:A:392:VAL:O	2:B:29:LEU:HD13	2.22	0.40
3:G:86:HIS:HD2	3:G:92:SER:HB2	1.85	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	603/649 (93%)	510 (85%)	77 (13%)	16 (3%)	5	35
1	E	603/649 (93%)	512 (85%)	77 (13%)	14 (2%)	6	38
2	B	250/296 (84%)	194 (78%)	44 (18%)	12 (5%)	2	24
2	F	250/296 (84%)	195 (78%)	42 (17%)	13 (5%)	2	23
3	C	176/204 (86%)	158 (90%)	17 (10%)	1 (1%)	25	62
3	G	176/204 (86%)	157 (89%)	18 (10%)	1 (1%)	25	62
4	D	46/123 (37%)	39 (85%)	5 (11%)	2 (4%)	2	26
4	H	46/123 (37%)	39 (85%)	5 (11%)	2 (4%)	2	26
All	All	2150/2544 (84%)	1804 (84%)	285 (13%)	61 (3%)	5	35

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	SER
1	A	222	PRO
1	A	239	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	548	ASN
2	B	279	PRO
2	F	97	PRO
2	F	101	LYS
2	F	125	ASP
1	E	178	SER
1	E	222	PRO
1	E	239	PHE
1	E	548	ASN
1	A	555	VAL
1	A	583	PRO
2	B	99	ALA
2	B	125	ASP
4	H	69	GLU
2	F	279	PRO
1	E	555	VAL
1	A	130	ARG
1	A	221	MET
1	A	306	LEU
1	A	338	ALA
1	A	410	TYR
1	A	570	GLU
2	B	242	PHE
3	C	124	GLU
4	D	69	GLU
2	F	216	THR
2	F	242	PHE
2	F	281	GLU
2	F	283	VAL
1	E	48	ILE
1	E	130	ARG
1	E	221	MET
1	E	583	PRO
1	A	48	ILE
2	B	97	PRO
2	B	192	GLU
2	B	273	PRO
2	B	281	GLU
2	F	192	GLU
2	F	240	LEU
1	E	306	LEU
1	E	338	ALA

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Mol	Chain	Res	Type
1	E	410	TYR
1	E	570	GLU
2	B	84	VAL
2	B	240	LEU
2	B	283	VAL
4	D	72	THR
3	G	124	GLU
4	H	72	THR
2	F	84	VAL
2	F	273	PRO
1	A	549	PHE
2	B	278	ASP
1	A	474	GLY
1	E	474	GLY
2	F	278	ASP
1	A	326	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	512/552 (93%)	482 (94%)	30 (6%)	19	51
1	E	512/552 (93%)	484 (94%)	28 (6%)	21	53
2	B	230/263 (88%)	195 (85%)	35 (15%)	3	18
2	F	230/263 (88%)	211 (92%)	19 (8%)	11	40
3	C	151/171 (88%)	143 (95%)	8 (5%)	22	54
3	G	151/171 (88%)	144 (95%)	7 (5%)	27	56
4	D	38/59 (64%)	34 (90%)	4 (10%)	7	30
4	H	38/59 (64%)	36 (95%)	2 (5%)	22	54
All	All	1862/2090 (89%)	1729 (93%)	133 (7%)	14	45

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	TYR
1	A	70	ARG
1	A	99	PHE
1	A	106	MET
1	A	114	PHE
1	A	139	ASN
1	A	145	PHE
1	A	151	LEU
1	A	156	PHE
1	A	166	TRP
1	A	172	LEU
1	A	175	ASN
1	A	210	LYS
1	A	216	MET
1	A	239	PHE
1	A	260	PHE
1	A	273	ASN
1	A	283	VAL
1	A	310	LYS
1	A	328	THR
1	A	329	HIS
1	A	363	LEU
1	A	395	VAL
1	A	416	PHE
1	A	432	PHE
1	A	436	TYR
1	A	500	PHE
1	A	552	LEU
1	A	581	HIS
1	A	633	TYR
2	B	20	LEU
2	B	27	PHE
2	B	29	LEU
2	B	39	PHE
2	B	98	GLU
2	B	101	LYS
2	B	103	LYS
2	B	115	TRP
2	B	125	ASP
2	B	129	VAL
2	B	134	ILE
2	B	140	ILE
2	B	148	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	153	LEU
2	B	161	GLN
2	B	169	LEU
2	B	171	ASP
2	B	175	GLN
2	B	188	ASN
2	B	193	HIS
2	B	194	PHE
2	B	200	ASP
2	B	208	ASP
2	B	213	VAL
2	B	214	LYS
2	B	215	LYS
2	B	216	THR
2	B	217	GLN
2	B	224	THR
2	B	228	TYR
2	B	232	MET
2	B	237	VAL
2	B	252	HIS
2	B	272	SER
2	B	277	THR
3	C	25	LEU
3	C	61	LEU
3	C	72	PHE
3	C	75	LEU
3	C	79	PHE
3	C	128	LEU
3	C	161	GLN
3	C	189	TRP
4	D	62	PHE
4	D	69	GLU
4	D	79	LEU
4	D	80	PHE
3	G	61	LEU
3	G	72	PHE
3	G	75	LEU
3	G	79	PHE
3	G	128	LEU
3	G	161	GLN
3	G	189	TRP
4	H	69	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	H	79	LEU
2	F	22	LEU
2	F	28	MET
2	F	29	LEU
2	F	39	PHE
2	F	115	TRP
2	F	153	LEU
2	F	165	MET
2	F	175	GLN
2	F	181	THR
2	F	188	ASN
2	F	208	ASP
2	F	213	VAL
2	F	223	LEU
2	F	224	THR
2	F	232	MET
2	F	237	VAL
2	F	246	HIS
2	F	272	SER
2	F	283	VAL
1	E	36	TYR
1	E	70	ARG
1	E	99	PHE
1	E	114	PHE
1	E	115	LEU
1	E	139	ASN
1	E	145	PHE
1	E	151	LEU
1	E	156	PHE
1	E	166	TRP
1	E	172	LEU
1	E	216	MET
1	E	239	PHE
1	E	260	PHE
1	E	273	ASN
1	E	283	VAL
1	E	288	LEU
1	E	310	LYS
1	E	328	THR
1	E	395	VAL
1	E	415	HIS
1	E	416	PHE

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Mol	Chain	Res	Type
1	E	432	PHE
1	E	436	TYR
1	E	500	PHE
1	E	552	LEU
1	E	581	HIS
1	E	633	TYR

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	53	HIS
1	A	329	HIS
2	B	217	GLN
2	B	246	HIS
2	B	252	HIS
1	E	53	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	HEA	E	1002	-	57,67,67	2.12	17 (29%)	61,103,103	2.50	25 (40%)
5	HEA	A	1001	1	57,67,67	2.25	19 (33%)	61,103,103	2.38	23 (37%)
7	IHQ	E	1004	-	12,15,21	1.89	2 (16%)	12,22,28	1.59	3 (25%)
7	IHQ	A	1004	-	12,15,21	1.92	2 (16%)	12,22,28	1.54	3 (25%)
5	HEA	A	1002	-	57,67,67	2.12	17 (29%)	61,103,103	2.52	25 (40%)
5	HEA	E	1001	1	57,67,67	2.25	19 (33%)	61,103,103	2.36	24 (39%)

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	HEA	E	1002	-	-	7/32/76/76	-
5	HEA	A	1001	1	-	8/32/76/76	-
7	IHQ	E	1004	-	-	-	0/2/2/2
7	IHQ	A	1004	-	-	-	0/2/2/2
5	HEA	A	1002	-	-	7/32/76/76	-
5	HEA	E	1001	1	-	8/32/76/76	-

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	HEA	C3A-C2A	5.98	1.48	1.40
5	E	1001	HEA	C3A-C2A	5.94	1.48	1.40
5	E	1001	HEA	C3B-C2B	5.83	1.47	1.34
5	A	1001	HEA	C3B-C2B	5.73	1.47	1.34
5	A	1002	HEA	C3B-C2B	5.55	1.47	1.34
5	E	1002	HEA	C3B-C2B	5.54	1.47	1.34
5	E	1002	HEA	C3A-C2A	5.52	1.48	1.40
5	A	1002	HEA	C3A-C2A	5.49	1.48	1.40
5	E	1001	HEA	C3C-C2C	5.46	1.47	1.40
5	A	1001	HEA	C3C-C2C	5.40	1.47	1.40
5	A	1001	HEA	C3D-C2D	5.27	1.47	1.36
7	A	1004	IHQ	C6-C5	5.23	1.49	1.41
5	A	1001	HEA	CHD-C1D	5.21	1.48	1.35
5	E	1001	HEA	C3D-C2D	5.20	1.47	1.36
7	E	1004	IHQ	C6-C5	5.19	1.49	1.41
5	E	1001	HEA	CHD-C1D	5.15	1.48	1.35
5	E	1001	HEA	CHC-C4B	5.11	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	HEA	CHC-C4B	5.11	1.48	1.35
5	E	1002	HEA	C3D-C2D	5.06	1.47	1.36
5	A	1002	HEA	C3D-C2D	5.03	1.47	1.36
5	A	1002	HEA	C3C-C2C	4.83	1.47	1.40
5	A	1002	HEA	CHC-C4B	4.83	1.47	1.35
5	E	1002	HEA	CHC-C4B	4.78	1.47	1.35
5	E	1002	HEA	C3C-C2C	4.78	1.47	1.40
5	E	1002	HEA	CHD-C1D	4.77	1.47	1.35
5	A	1002	HEA	CHD-C1D	4.76	1.47	1.35
7	A	1004	IHQ	O11-N10	3.26	1.44	1.39
5	E	1001	HEA	C2A-C1A	3.23	1.49	1.42
7	E	1004	IHQ	O11-N10	3.19	1.43	1.39
5	A	1001	HEA	C2A-C1A	3.17	1.49	1.42
5	A	1002	HEA	C2A-C1A	3.12	1.49	1.42
5	A	1002	HEA	FE-ND	3.11	2.12	1.96
5	E	1002	HEA	FE-ND	3.11	2.12	1.96
5	E	1002	HEA	FE-NB	3.11	2.12	1.96
5	A	1002	HEA	FE-NB	3.05	2.11	1.96
5	E	1002	HEA	C2A-C1A	3.02	1.49	1.42
5	E	1001	HEA	C1D-ND	-2.95	1.35	1.40
5	A	1001	HEA	C1D-ND	-2.91	1.35	1.40
5	E	1001	HEA	C4B-NB	-2.90	1.35	1.40
5	A	1001	HEA	C4B-NB	-2.89	1.35	1.40
5	E	1001	HEA	FE-ND	2.87	2.11	1.96
5	A	1001	HEA	FE-ND	2.87	2.11	1.96
5	A	1001	HEA	C4B-C3B	2.86	1.49	1.44
5	E	1001	HEA	C4B-C3B	2.83	1.49	1.44
5	A	1001	HEA	FE-NB	2.77	2.10	1.96
5	E	1001	HEA	FE-NB	2.75	2.10	1.96
5	E	1002	HEA	C4B-C3B	2.74	1.49	1.44
5	E	1002	HEA	C1D-ND	-2.72	1.35	1.40
5	A	1002	HEA	C1D-ND	-2.71	1.35	1.40
5	E	1002	HEA	C4B-NB	-2.71	1.35	1.40
5	A	1002	HEA	C4B-C3B	2.68	1.49	1.44
5	A	1002	HEA	C4B-NB	-2.68	1.35	1.40
5	E	1001	HEA	C1C-CHC	2.55	1.48	1.41
5	A	1001	HEA	C4C-CHD	2.53	1.48	1.41
5	E	1001	HEA	C1D-C2D	2.53	1.49	1.44
5	E	1001	HEA	C4C-CHD	2.53	1.48	1.41
5	A	1001	HEA	C1C-CHC	2.51	1.48	1.41
5	E	1002	HEA	C1D-C2D	2.44	1.49	1.44
5	A	1001	HEA	C1D-C2D	2.42	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1001	HEA	CHB-C1B	2.36	1.47	1.41
5	A	1002	HEA	C1D-C2D	2.33	1.49	1.44
5	A	1001	HEA	CHB-C1B	2.33	1.47	1.41
5	E	1002	HEA	C1B-C2B	2.31	1.49	1.44
5	A	1001	HEA	C4D-C3D	2.30	1.49	1.45
5	E	1002	HEA	C4D-C3D	2.30	1.49	1.45
5	E	1002	HEA	C1C-CHC	2.25	1.47	1.41
5	E	1002	HEA	C4C-CHD	2.25	1.47	1.41
5	A	1002	HEA	C4D-C3D	2.25	1.48	1.45
5	E	1001	HEA	C4D-C3D	2.24	1.48	1.45
5	A	1001	HEA	C1B-C2B	2.23	1.48	1.44
5	E	1001	HEA	C1B-C2B	2.21	1.48	1.44
5	A	1002	HEA	C4C-CHD	2.20	1.47	1.41
5	A	1002	HEA	C1B-C2B	2.20	1.48	1.44
5	A	1002	HEA	C1C-CHC	2.19	1.47	1.41
5	A	1001	HEA	CHA-C4D	2.11	1.47	1.41
5	E	1001	HEA	CHA-C4D	2.06	1.47	1.41

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1002	HEA	C3D-C4D-ND	7.15	117.28	110.36
5	E	1002	HEA	C3D-C4D-ND	6.97	117.11	110.36
5	A	1001	HEA	CHA-C4D-ND	-6.13	117.78	124.43
5	E	1001	HEA	CHA-C4D-ND	-6.04	117.87	124.43
5	E	1001	HEA	C3D-C4D-ND	5.93	116.10	110.36
5	A	1001	HEA	C3D-C4D-ND	5.79	115.97	110.36
5	E	1002	HEA	C2B-C1B-NB	5.73	116.75	109.88
5	A	1002	HEA	C2B-C1B-NB	5.65	116.66	109.88
5	A	1002	HEA	C2D-C1D-ND	5.54	116.40	109.84
5	E	1002	HEA	C2D-C1D-ND	5.48	116.33	109.84
5	A	1001	HEA	C4D-CHA-C1A	-5.46	115.35	122.56
5	E	1002	HEA	C3B-C4B-NB	5.43	116.27	109.84
5	E	1001	HEA	C4D-CHA-C1A	-5.25	115.63	122.56
5	A	1002	HEA	C3B-C4B-NB	5.15	115.94	109.84
5	A	1002	HEA	CHA-C4D-ND	-4.47	119.57	124.43
5	A	1001	HEA	C2D-C1D-ND	4.36	115.00	109.84
5	E	1001	HEA	C2D-C1D-ND	4.31	114.95	109.84
5	A	1001	HEA	C3B-C4B-NB	4.29	114.92	109.84
5	E	1001	HEA	C3B-C4B-NB	4.27	114.90	109.84
5	A	1001	HEA	C2B-C1B-NB	4.26	114.99	109.88
5	E	1001	HEA	C2B-C1B-NB	4.23	114.95	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1002	HEA	C1D-C2D-C3D	-4.23	102.51	106.96
5	E	1002	HEA	C1D-C2D-C3D	-4.20	102.54	106.96
5	E	1002	HEA	CHA-C4D-ND	-4.11	119.96	124.43
5	A	1002	HEA	C3C-C4C-NC	4.09	114.50	109.21
5	E	1002	HEA	C3C-C4C-NC	3.95	114.31	109.21
5	A	1002	HEA	C1B-C2B-C3B	-3.93	102.10	106.80
5	E	1002	HEA	C1B-C2B-C3B	-3.91	102.13	106.80
5	A	1001	HEA	C1D-C2D-C3D	-3.75	103.01	106.96
5	E	1001	HEA	C1D-C2D-C3D	-3.73	103.04	106.96
5	A	1001	HEA	CMC-C2C-C3C	3.57	131.35	124.68
7	A	1004	IHQ	C6-C5-N10	3.54	121.01	117.65
5	A	1002	HEA	C4D-C3D-C2D	-3.51	101.78	106.90
7	E	1004	IHQ	C6-C5-N10	3.46	120.93	117.65
5	E	1002	HEA	C4D-C3D-C2D	-3.44	101.88	106.90
5	A	1002	HEA	CMC-C2C-C3C	3.40	131.04	124.68
5	E	1002	HEA	CMC-C2C-C3C	3.39	131.02	124.68
5	E	1001	HEA	C4D-C3D-C2D	-3.34	102.03	106.90
5	A	1001	HEA	C4D-C3D-C2D	-3.32	102.06	106.90
5	E	1001	HEA	C3C-C4C-NC	3.30	113.48	109.21
5	E	1001	HEA	CMC-C2C-C3C	3.27	130.79	124.68
5	A	1002	HEA	C13-C14-C15	-3.24	119.85	127.66
7	E	1004	IHQ	C13-C9-C8	-3.23	118.12	123.77
5	A	1001	HEA	CHB-C1B-NB	-3.22	120.94	124.43
5	E	1002	HEA	CHB-C1B-NB	-3.20	120.95	124.43
5	E	1001	HEA	C1B-C2B-C3B	-3.17	103.02	106.80
5	A	1001	HEA	C1B-C2B-C3B	-3.16	103.02	106.80
5	A	1001	HEA	C3C-C4C-NC	3.16	113.29	109.21
5	E	1002	HEA	C26-C15-C16	3.11	120.50	115.27
5	E	1001	HEA	C26-C15-C16	3.07	120.43	115.27
5	A	1002	HEA	C26-C15-C16	3.03	120.37	115.27
5	E	1001	HEA	CHB-C1B-NB	-3.02	121.15	124.43
5	A	1001	HEA	C26-C15-C16	3.01	120.33	115.27
5	E	1001	HEA	C17-C18-C19	-3.00	120.44	127.66
5	A	1002	HEA	C27-C19-C20	2.97	120.27	115.27
5	A	1002	HEA	C1D-ND-C4D	-2.96	102.02	105.07
5	E	1002	HEA	C13-C14-C15	-2.89	120.71	127.66
5	A	1001	HEA	C17-C18-C19	-2.87	120.75	127.66
5	E	1001	HEA	C4B-C3B-C2B	-2.84	102.55	107.41
5	E	1002	HEA	C1D-ND-C4D	-2.84	102.14	105.07
5	E	1002	HEA	C4B-C3B-C2B	-2.83	102.58	107.41
5	A	1001	HEA	C4B-C3B-C2B	-2.82	102.60	107.41
5	A	1002	HEA	C17-C18-C19	-2.80	120.92	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1002	HEA	C13-C12-C11	-2.79	110.16	114.35
7	A	1004	IHQ	C13-C9-C8	-2.78	118.92	123.77
5	A	1001	HEA	CHC-C4B-NB	-2.77	120.96	124.38
5	A	1002	HEA	CHB-C1B-NB	-2.73	121.47	124.43
5	E	1001	HEA	CHC-C4B-NB	-2.73	121.01	124.38
5	E	1002	HEA	C4B-NB-C1B	-2.71	102.27	105.07
5	E	1002	HEA	C17-C18-C19	-2.71	121.13	127.66
5	A	1002	HEA	C4B-C3B-C2B	-2.70	102.80	107.41
5	E	1001	HEA	C27-C19-C20	2.67	119.75	115.27
5	E	1001	HEA	CMD-C2D-C1D	2.67	129.10	125.04
5	E	1002	HEA	CMB-C2B-C1B	2.66	129.09	125.04
5	A	1001	HEA	CAD-C3D-C4D	2.65	129.29	124.66
5	E	1001	HEA	CAD-C3D-C4D	2.60	129.20	124.66
5	E	1002	HEA	C27-C19-C20	2.60	119.64	115.27
5	A	1001	HEA	CMB-C2B-C1B	2.54	128.91	125.04
5	A	1002	HEA	CMB-C2B-C1B	2.53	128.90	125.04
5	A	1001	HEA	C27-C19-C20	2.51	119.49	115.27
5	A	1002	HEA	C4B-NB-C1B	-2.49	102.50	105.07
5	A	1002	HEA	C25-C23-C24	2.47	120.06	114.60
5	A	1001	HEA	CMD-C2D-C1D	2.42	128.73	125.04
5	E	1001	HEA	C25-C23-C24	2.41	119.93	114.60
5	E	1002	HEA	C25-C23-C24	2.40	119.91	114.60
5	E	1002	HEA	CAD-C3D-C4D	2.38	128.82	124.66
5	E	1001	HEA	CMB-C2B-C1B	2.35	128.61	125.04
5	E	1002	HEA	CMD-C2D-C1D	2.32	128.57	125.04
5	E	1002	HEA	CBA-CAA-C2A	-2.30	108.72	112.60
5	A	1001	HEA	C25-C23-C24	2.30	119.68	114.60
5	A	1001	HEA	C13-C14-C15	-2.26	122.23	127.66
5	A	1002	HEA	CAD-C3D-C4D	2.25	128.60	124.66
5	E	1001	HEA	CHD-C1D-ND	-2.20	121.66	124.38
5	A	1002	HEA	CMD-C2D-C1D	2.16	128.33	125.04
5	E	1002	HEA	C13-C12-C11	-2.15	111.12	114.35
7	A	1004	IHQ	C5-C6-C7	-2.15	119.28	121.44
5	A	1002	HEA	CHD-C1D-C2D	-2.13	120.83	126.72
5	E	1001	HEA	C13-C14-C15	-2.10	122.59	127.66
5	E	1002	HEA	CHD-C1D-C2D	-2.10	120.91	126.72
7	E	1004	IHQ	C5-C6-C7	-2.05	119.38	121.44
5	A	1001	HEA	CHD-C1D-ND	-2.05	121.85	124.38
5	A	1002	HEA	CAD-CBD-CGD	-2.04	109.21	113.60
5	E	1001	HEA	C21-C22-C23	-2.00	120.91	127.75

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	HEA	C3B-C11-C12-C13
5	A	1001	HEA	O11-C11-C12-C13
5	E	1001	HEA	C3B-C11-C12-C13
5	E	1001	HEA	O11-C11-C12-C13
5	A	1001	HEA	C15-C16-C17-C18
5	E	1001	HEA	C15-C16-C17-C18
5	A	1001	HEA	C26-C15-C16-C17
5	E	1001	HEA	C26-C15-C16-C17
5	A	1001	HEA	C14-C15-C16-C17
5	E	1001	HEA	C14-C15-C16-C17
5	A	1002	HEA	CAD-CBD-CGD-O1D
5	E	1002	HEA	CAD-CBD-CGD-O1D
5	A	1002	HEA	C4D-C3D-CAD-CBD
5	A	1002	HEA	C2D-C3D-CAD-CBD
5	E	1002	HEA	CAD-CBD-CGD-O2D
5	A	1002	HEA	CAD-CBD-CGD-O2D
5	E	1002	HEA	C2D-C3D-CAD-CBD
5	E	1002	HEA	C4D-C3D-CAD-CBD
5	A	1001	HEA	CAD-CBD-CGD-O2D
5	E	1001	HEA	CAD-CBD-CGD-O2D
5	A	1002	HEA	C26-C15-C16-C17
5	E	1002	HEA	C26-C15-C16-C17
5	A	1002	HEA	CAA-CBA-CGA-O2A
5	E	1002	HEA	CAA-CBA-CGA-O2A
5	E	1002	HEA	CAA-CBA-CGA-O1A
5	A	1001	HEA	CAD-CBD-CGD-O1D
5	A	1002	HEA	CAA-CBA-CGA-O1A
5	E	1001	HEA	CAD-CBD-CGD-O1D
5	A	1001	HEA	CAA-CBA-CGA-O1A
5	E	1001	HEA	CAA-CBA-CGA-O1A

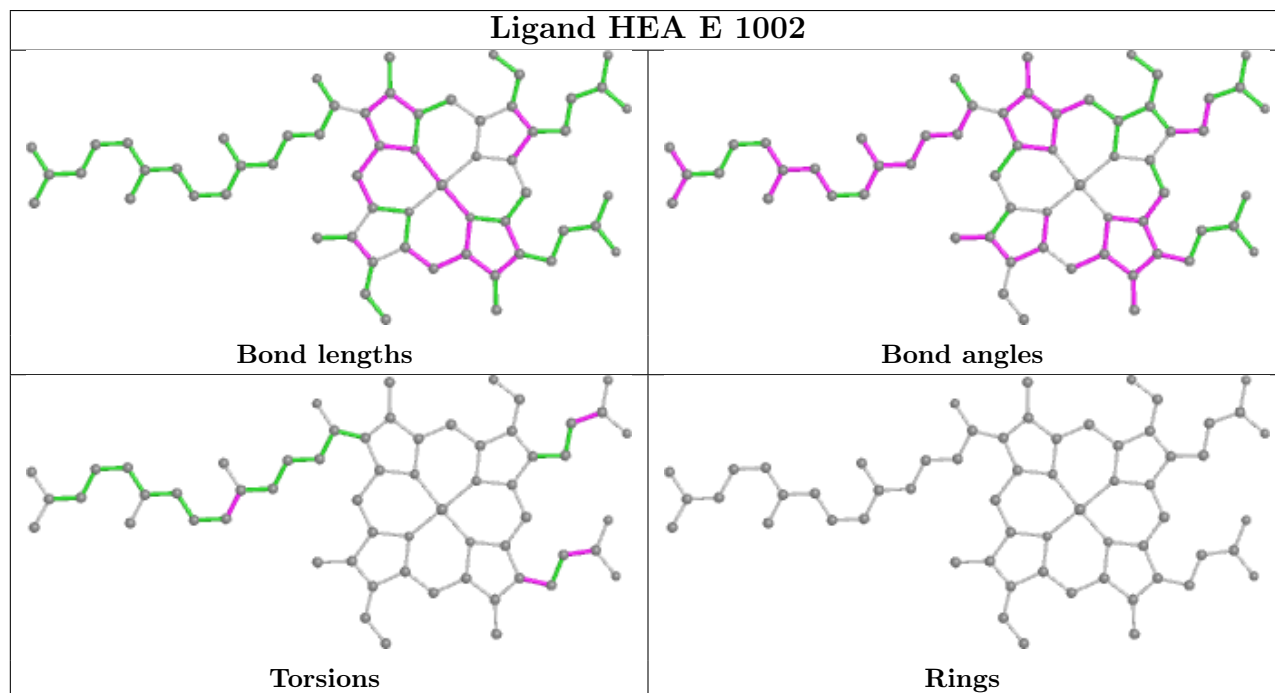
There are no ring outliers.

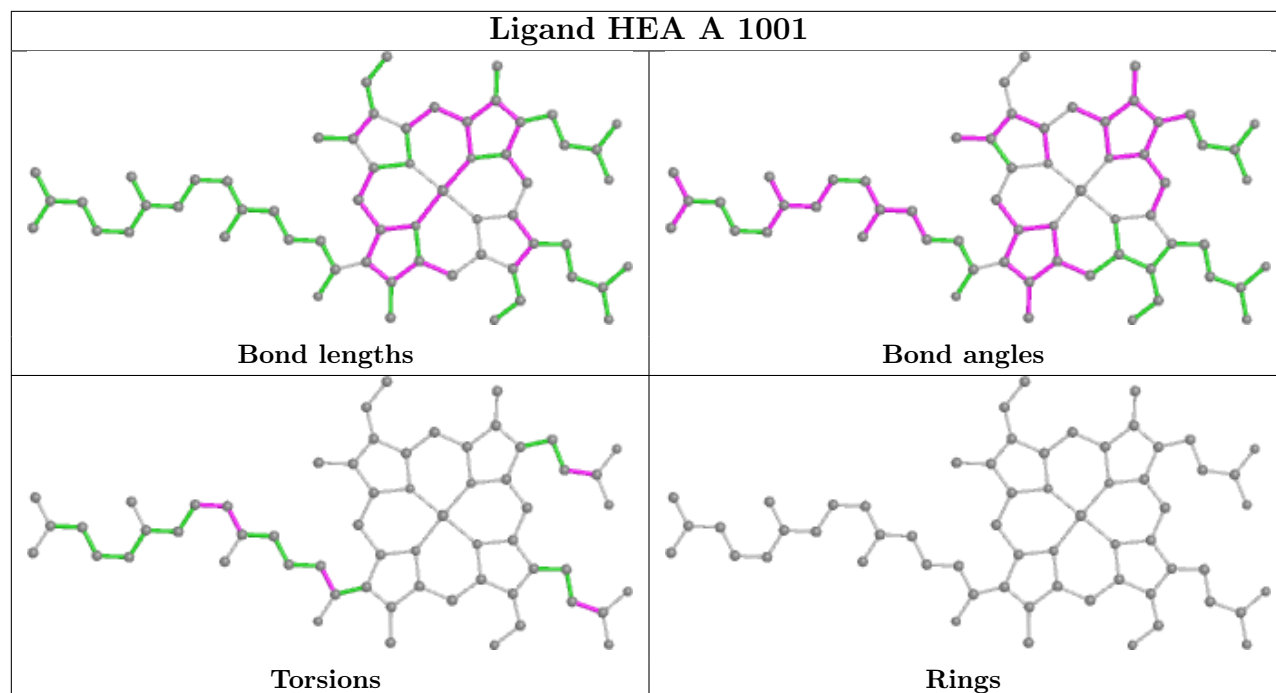
4 monomers are involved in 20 short contacts:

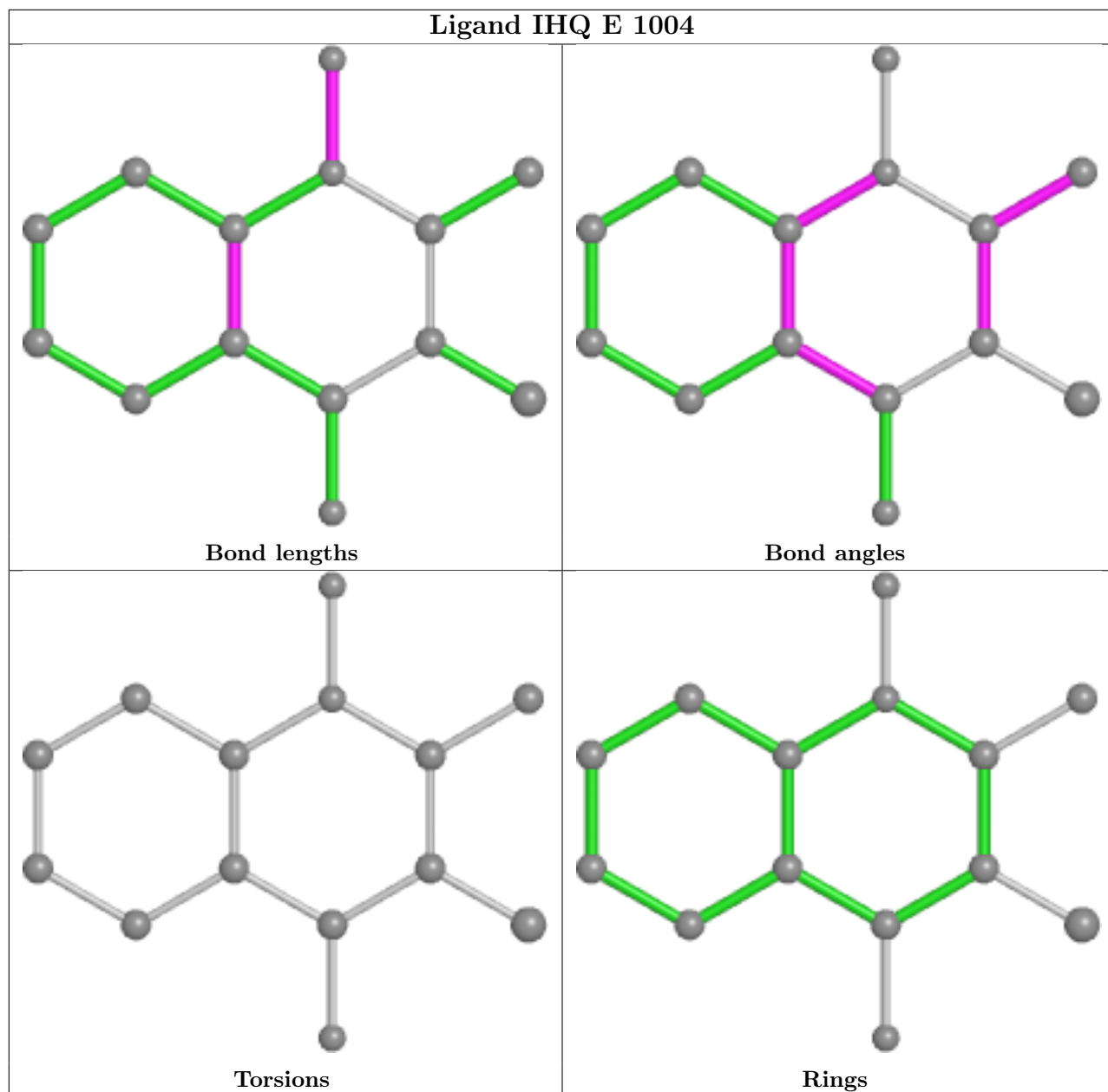
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1002	HEA	6	0
5	A	1001	HEA	5	0
5	A	1002	HEA	5	0
5	E	1001	HEA	4	0

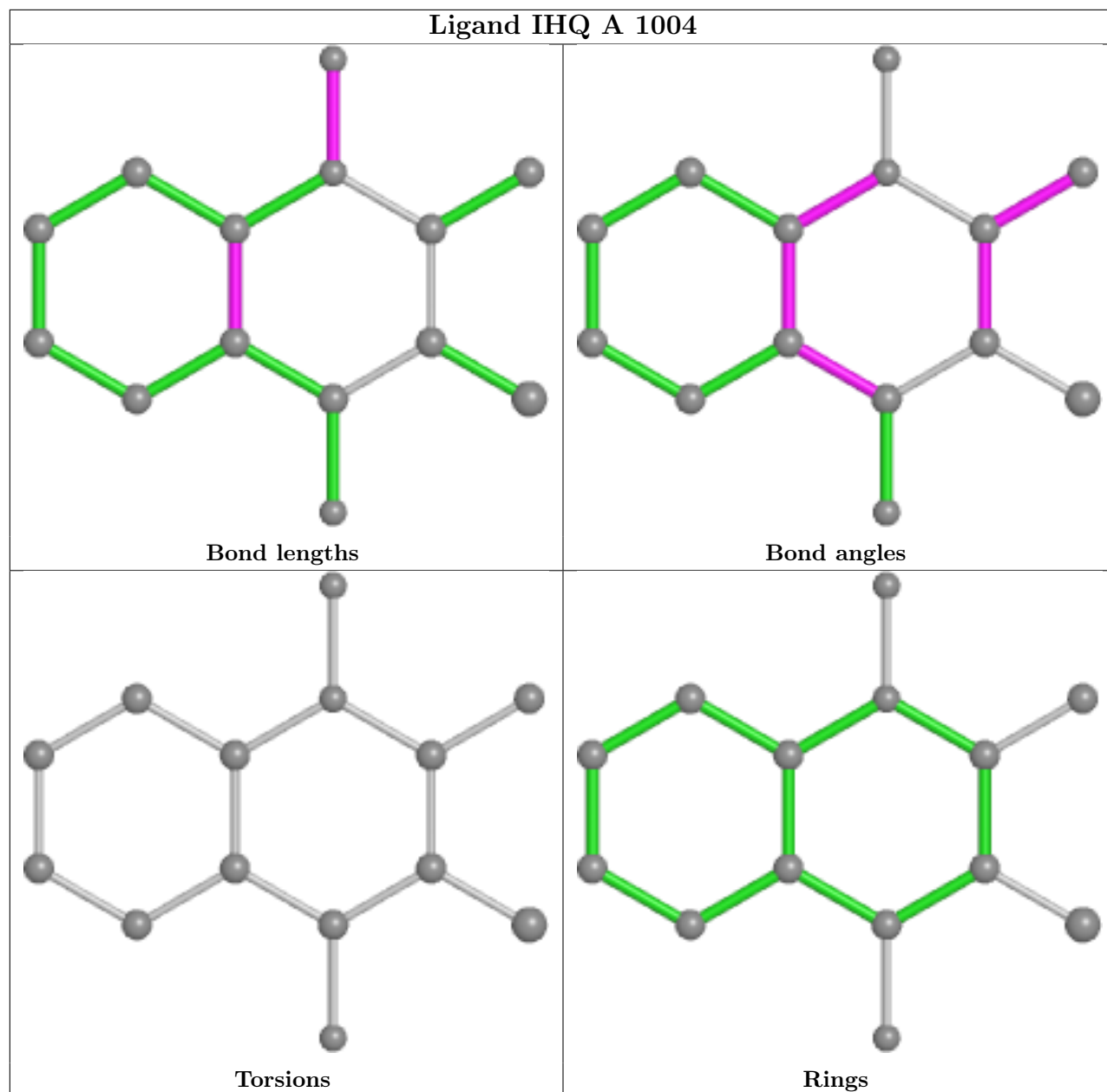
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

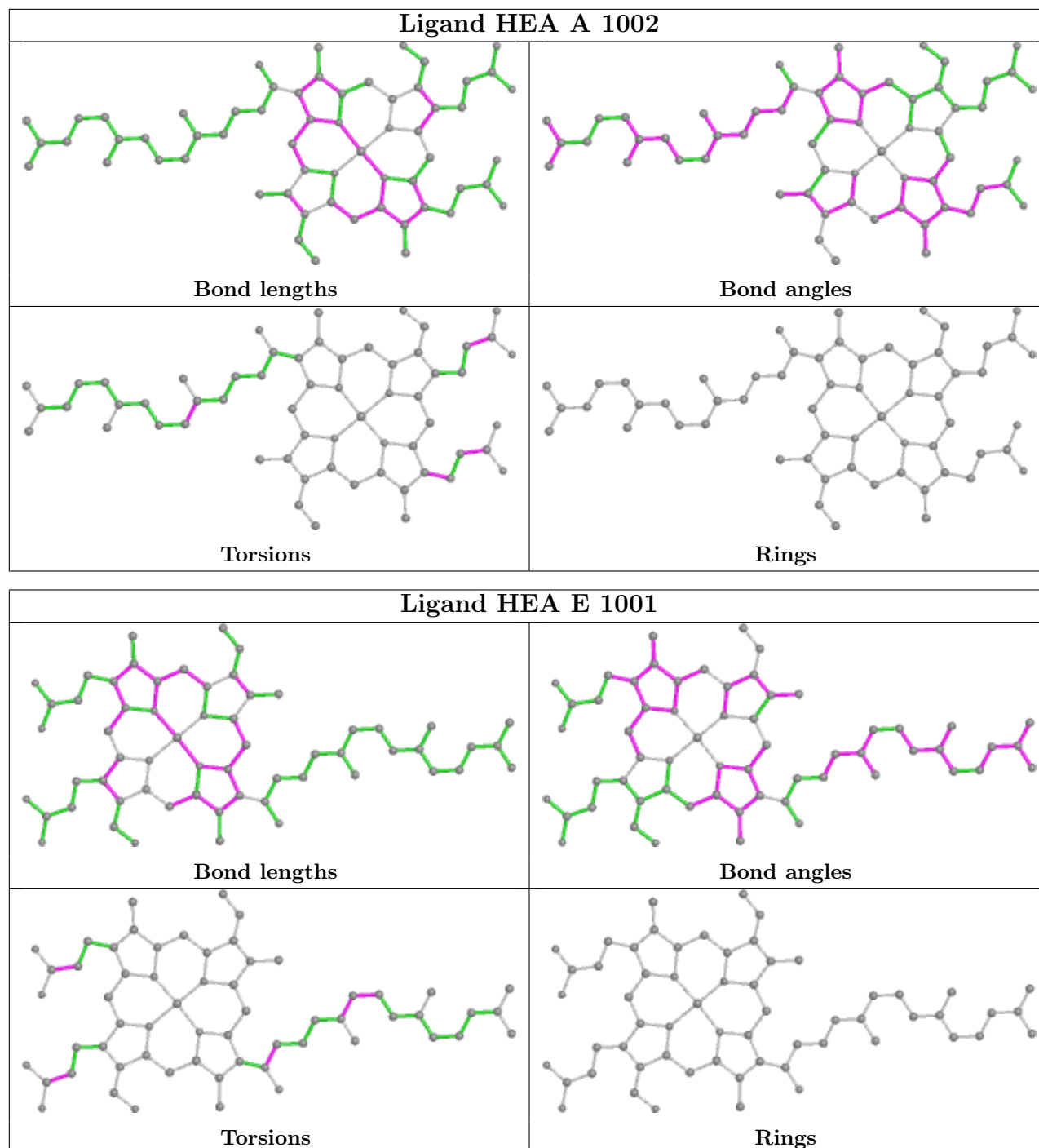












## 5.7 Other polymers [i](#)

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	607/649 (93%)	-0.04	20 (3%) 46 38	52, 115, 170, 235	0
1	E	607/649 (93%)	-0.00	22 (3%) 42 35	58, 117, 182, 232	0
2	B	256/296 (86%)	0.21	19 (7%) 14 11	71, 145, 209, 264	0
2	F	256/296 (86%)	0.10	15 (5%) 22 18	57, 142, 206, 254	0
3	C	178/204 (87%)	-0.16	6 (3%) 45 37	69, 122, 185, 208	0
3	G	178/204 (87%)	-0.00	13 (7%) 15 12	65, 125, 196, 241	0
4	D	48/123 (39%)	0.02	4 (8%) 11 9	73, 118, 172, 196	0
4	H	48/123 (39%)	-0.44	0 100 100	76, 117, 172, 180	0
All	All	2178/2544 (85%)	0.00	99 (4%) 33 28	52, 123, 190, 264	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	57	LEU	7.4
3	C	50	ASN	7.0
3	G	53	ALA	7.0
1	E	580	ILE	6.8
2	F	236	ASN	6.2
2	B	42	ILE	5.8
2	B	236	ASN	5.7
2	B	274	HIS	5.4
1	E	370	ARG	5.1
2	B	73	VAL	5.1
3	G	52	THR	5.0
1	A	550	ALA	4.9
1	E	213	THR	4.7
4	D	60	LEU	4.6
2	B	95	LYS	4.6
3	G	56	VAL	4.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	578	LYS	4.5
2	B	92	SER	4.2
2	B	97	PRO	4.1
1	A	86	ASN	4.0
1	E	333	THR	3.9
1	E	587	GLY	3.9
2	F	288	PHE	3.9
1	E	29	ALA	3.9
2	F	215	LYS	3.8
1	A	486	ASP	3.7
2	B	98	GLU	3.7
3	G	124	GLU	3.6
2	F	49	ARG	3.6
2	F	50	LYS	3.5
1	E	130	ARG	3.4
1	E	584	SER	3.4
1	A	541	SER	3.3
1	E	33	VAL	3.3
2	B	120	SER	3.2
3	G	90	ARG	3.2
1	E	366	MET	3.2
4	D	69	GLU	3.0
1	E	40	TRP	3.0
2	F	274	HIS	3.0
3	C	97	VAL	2.9
2	F	106	LEU	2.9
2	B	288	PHE	2.9
2	F	214	LYS	2.9
3	G	54	GLY	2.8
1	A	445	ASN	2.8
1	A	540	SER	2.8
3	G	50	ASN	2.8
2	F	277	THR	2.7
2	B	34	VAL	2.7
1	A	579	LYS	2.6
1	A	507	LEU	2.6
3	G	59	ASP	2.6
4	D	59	LEU	2.6
2	B	287	GLU	2.6
2	B	70	VAL	2.5
1	A	85	PRO	2.5
2	B	16	GLN	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	303	ARG	2.5
2	F	253	GLY	2.5
3	G	92	SER	2.5
3	G	89	ARG	2.5
1	A	48	ILE	2.5
3	G	58	PRO	2.5
2	B	282	ASN	2.4
3	C	163	LYS	2.4
1	E	372	SER	2.4
3	C	49	LYS	2.3
1	A	15	LEU	2.3
1	A	423	GLY	2.3
2	B	108	VAL	2.3
1	E	583	PRO	2.2
1	E	606	GLU	2.2
1	E	310	LYS	2.2
2	B	45	LYS	2.2
2	B	99	ALA	2.2
2	F	211	SER	2.2
1	A	606	GLU	2.2
1	E	34	LEU	2.2
1	A	448	ILE	2.2
1	E	32	PHE	2.2
3	G	91	GLY	2.2
1	A	441	GLY	2.1
2	F	81	ALA	2.1
1	A	87	ASN	2.1
2	F	287	GLU	2.1
1	E	279	GLY	2.1
2	B	38	LEU	2.1
1	A	424	THR	2.1
2	F	78	ILE	2.1
1	E	455	ILE	2.1
1	E	485	ASN	2.1
1	A	485	ASN	2.1
1	A	14	PRO	2.0
1	E	486	ASP	2.0
4	D	63	MET	2.0
2	F	48	ASP	2.0
3	C	77	SER	2.0
3	C	80	THR	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](#)

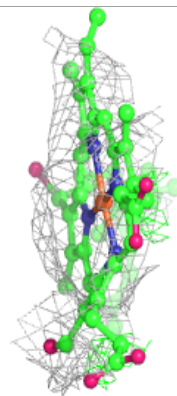
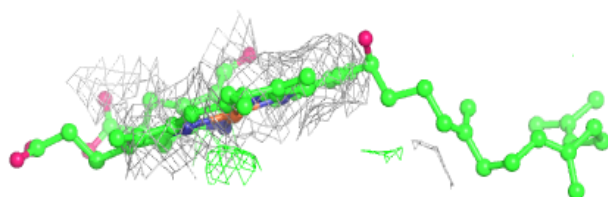
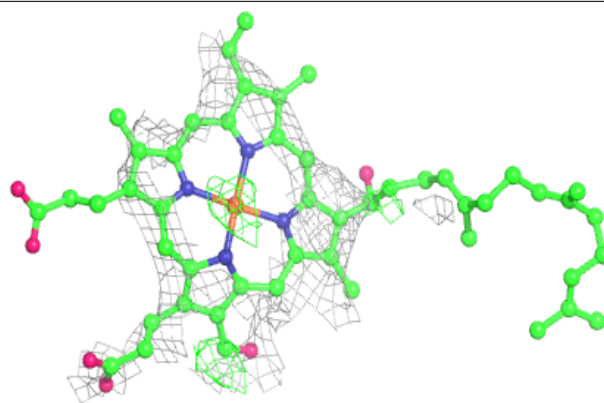
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	CU	A	1003	1/1	0.66	0.36	146,146,146,146	0
5	HEA	A	1002	60/60	0.79	0.43	100,143,198,223	0
5	HEA	E	1002	60/60	0.81	0.40	76,131,152,168	0
5	HEA	A	1001	60/60	0.81	0.42	80,129,190,212	0
5	HEA	E	1001	60/60	0.84	0.42	81,131,169,173	0
7	IHQ	E	1004	14/20	0.92	0.18	106,113,138,146	0
7	IHQ	A	1004	14/20	0.94	0.16	76,109,123,159	0
6	CU	E	1003	1/1	0.94	0.28	114,114,114,114	0

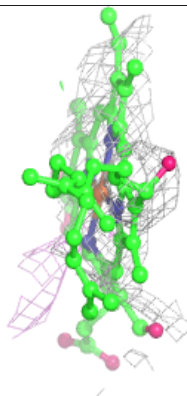
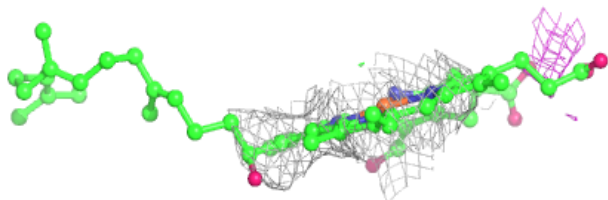
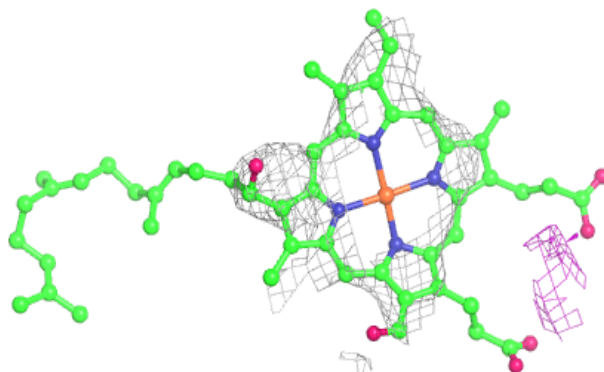
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around HEA A 1002:**

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

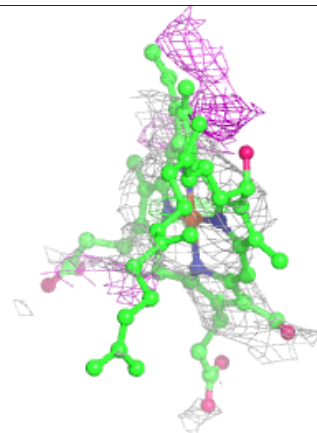
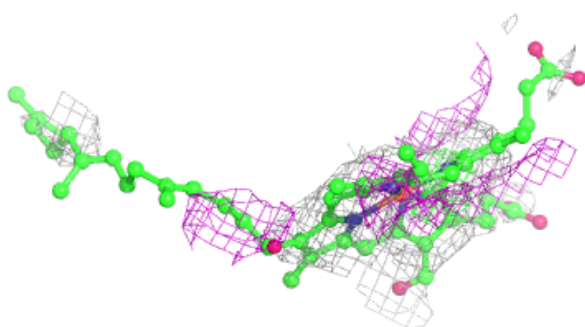
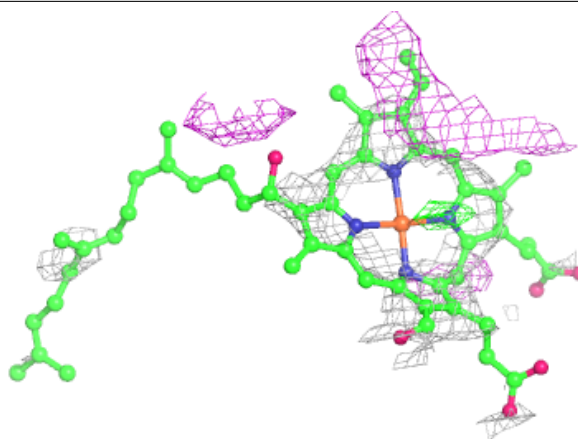
**Electron density around HEA E 1002:**

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

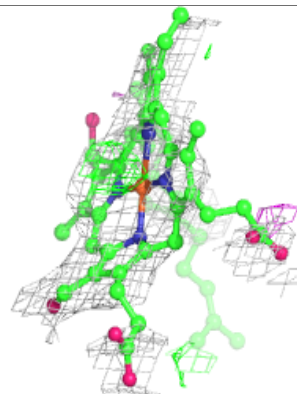
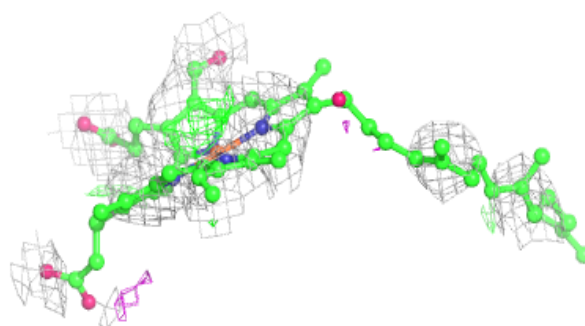
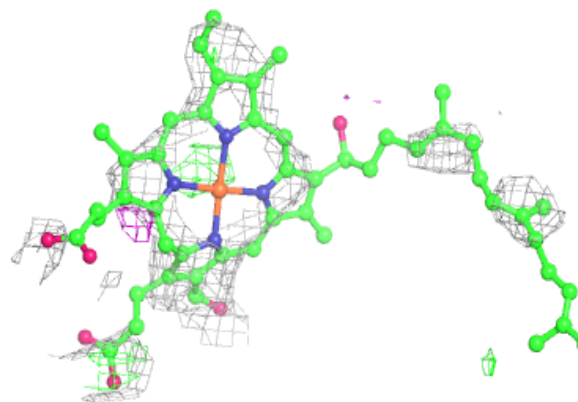


**Electron density around HEA A 1001:**

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

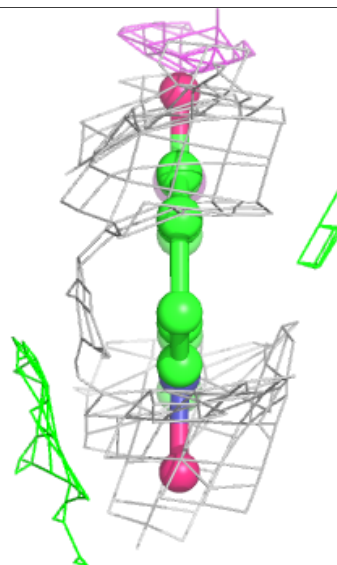
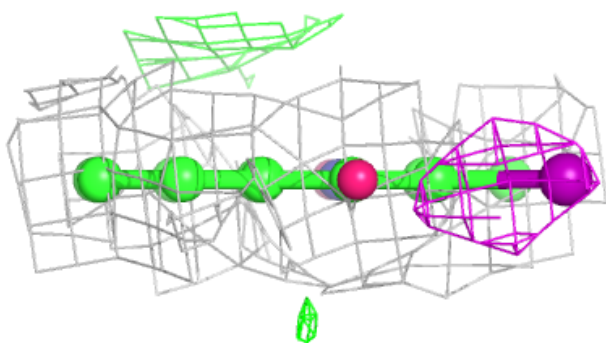
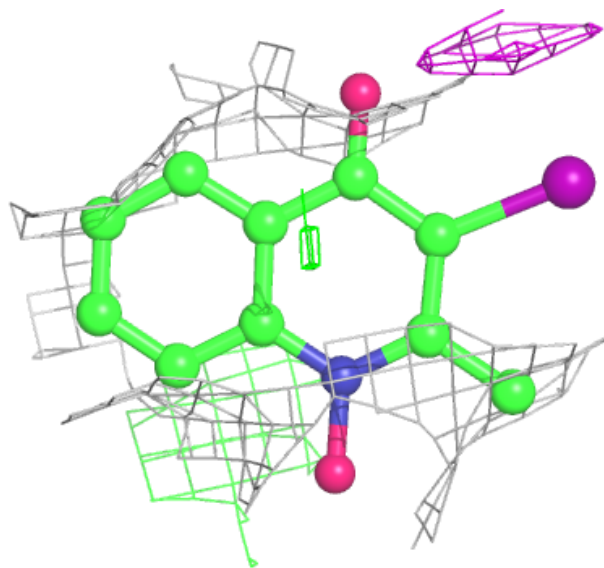
**Electron density around HEA E 1001:**

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

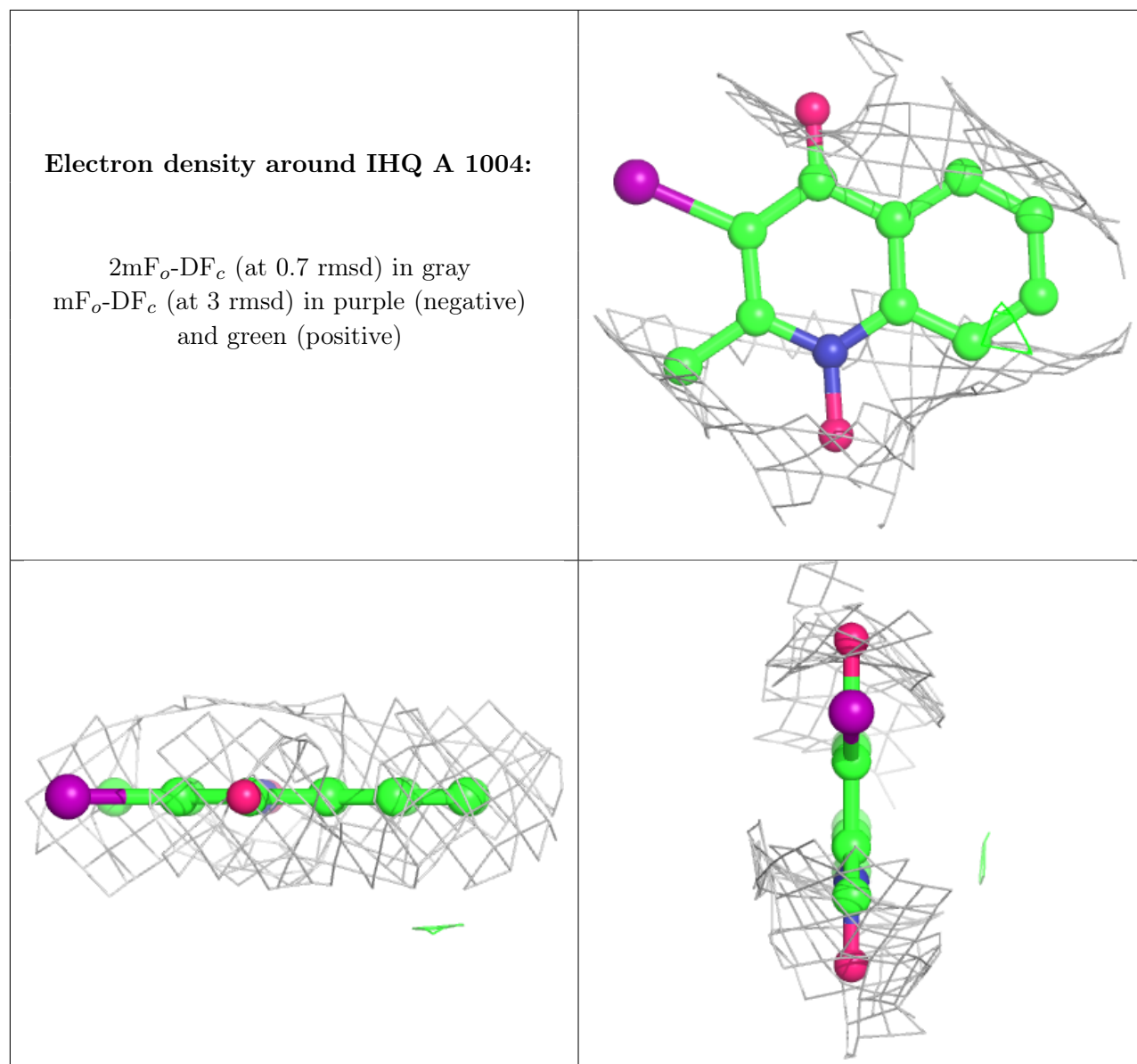


**Electron density around IHQ E 1004:**

$2mF_o-DF_c$  (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.