



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:46 AM UTC

PDB ID : 6KOC / pdb_00006koc
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

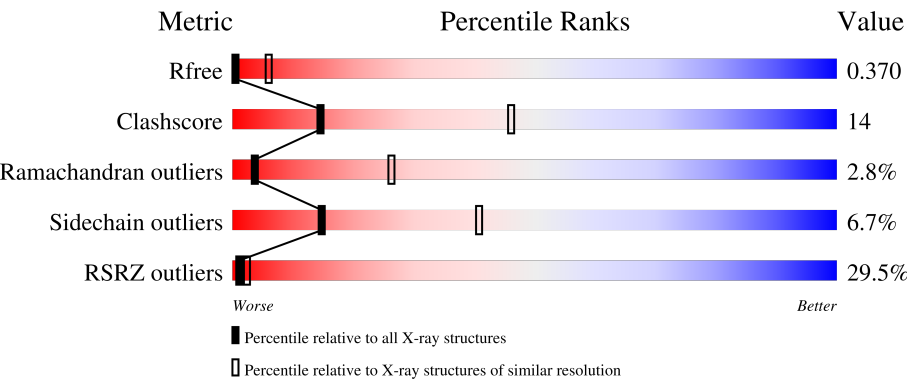
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	29% 58% 33% 6%
1	E	649	29% 63% 28% 6%
2	B	296	26% 43% 33% 9% 14%
2	F	296	25% 53% 27% 6% 14%

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Mol	Chain	Length	Quality of chain
3	C	204	22% 68% 18% • 13%
3	G	204	23% 70% 16% • 13%
4	D	123	13% 42% 14% • 43%
4	H	123	7% 46% 11% • 43%

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
1	A	607	Total	C	N	O	S	0	0	0
			4855	3270	752	792	41			
1	E	607	Total	C	N	O	S	0	0	0
			4855	3270	752	792	41			

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

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

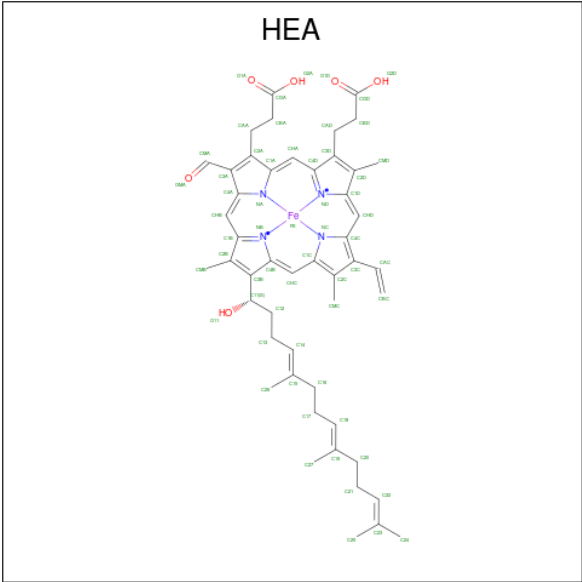
- Molecule 3 is a protein called AA3-600 quinol oxidase subunit IIII.

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

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

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

- Molecule 5 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).

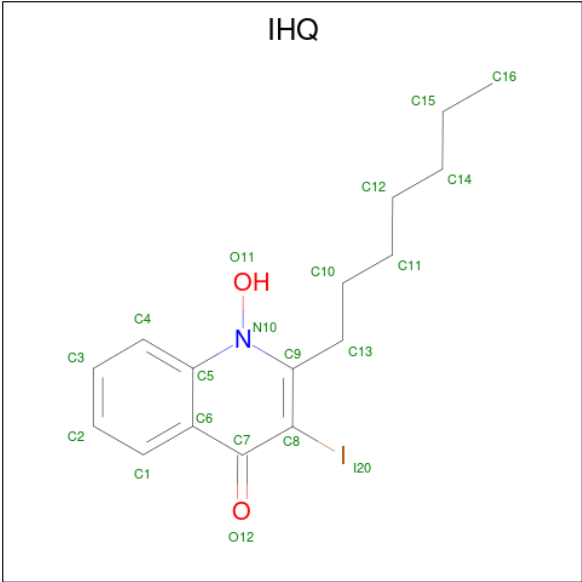


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
5	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
5	E	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
5	E	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 6 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 7 is 2-heptyl-3-iodanyl-1-oxidanyl-quinolin-4-one (CCD ID: IHQ) (formula: C₁₆H₂₀INO₂).

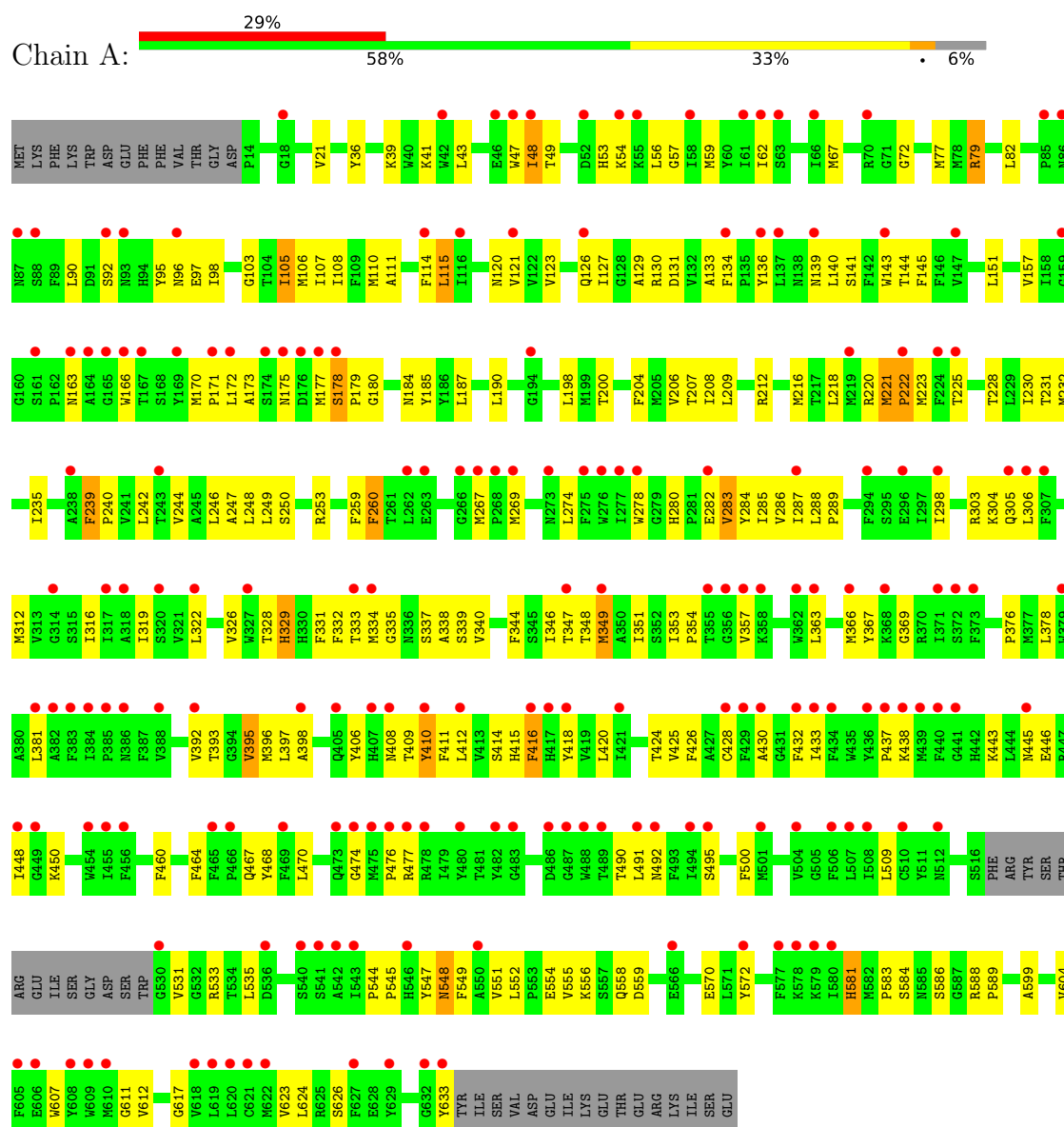


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	I	N	O	0	0
			14	10	1	1	2		
7	E	1	Total	C	I	N	O	0	0
			14	10	1	1	2		

3 Residue-property plots

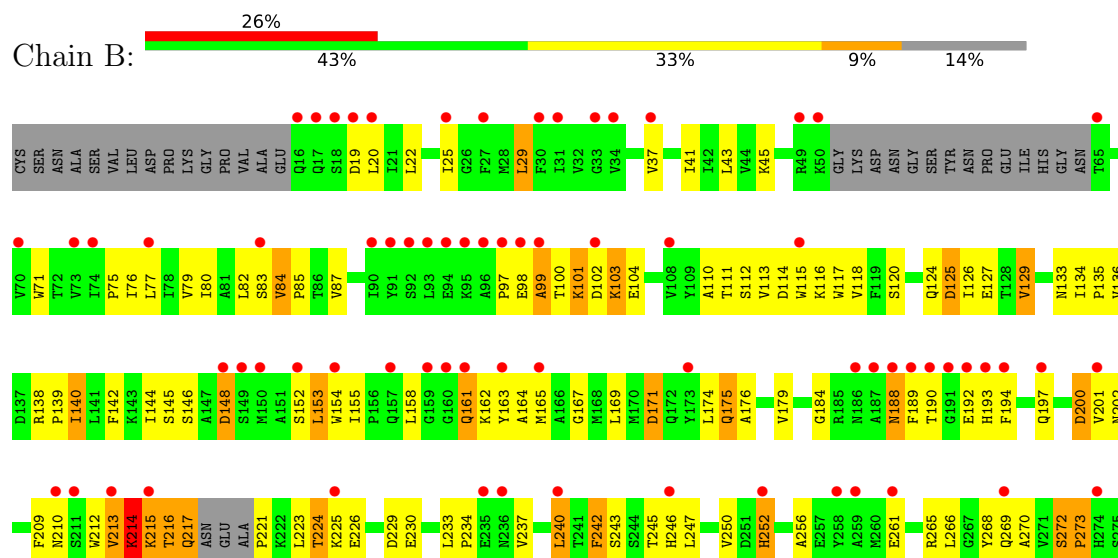
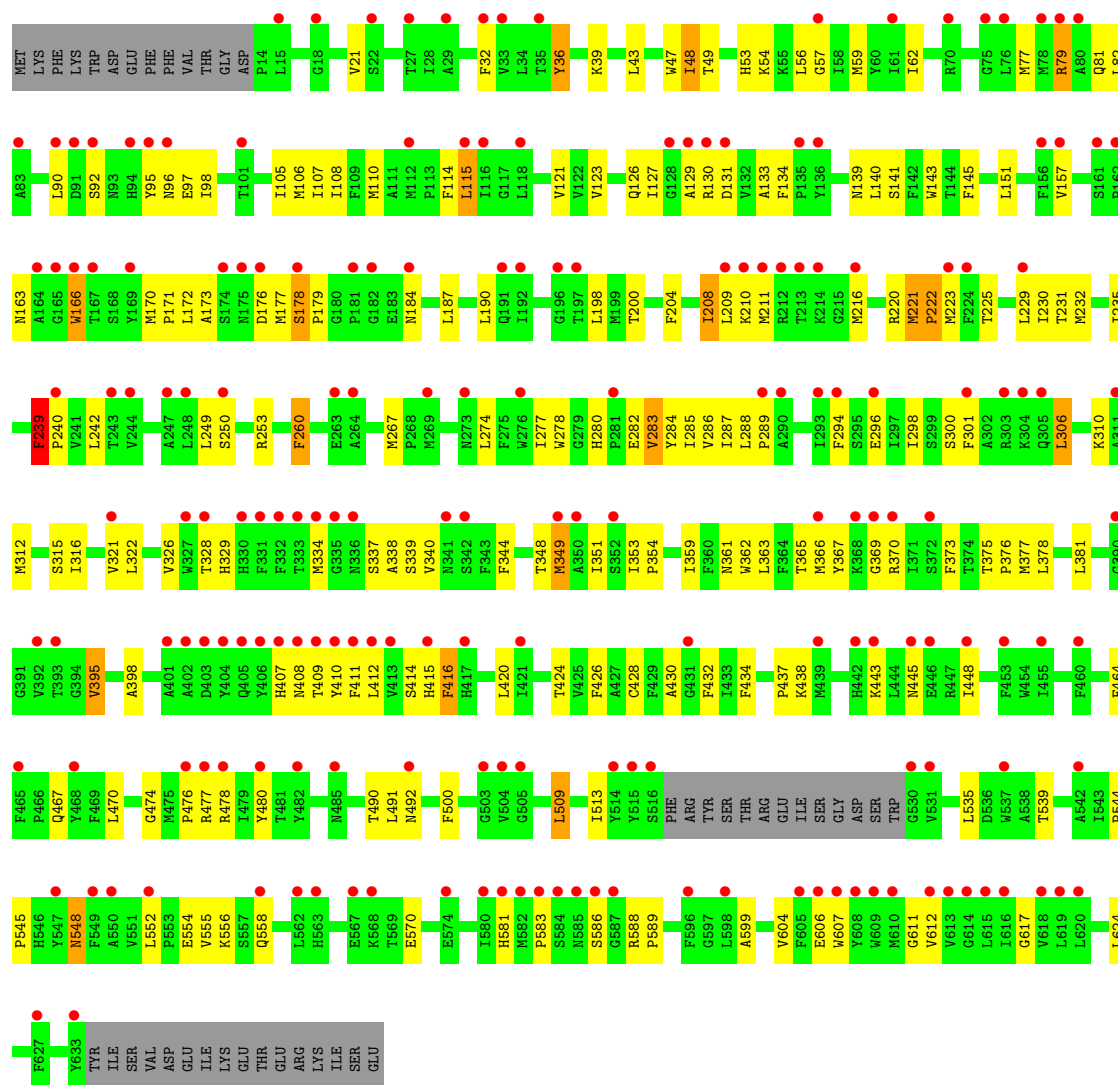
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

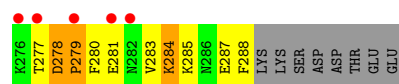
• Molecule 1: AA3-600 quinol oxidase subunit I



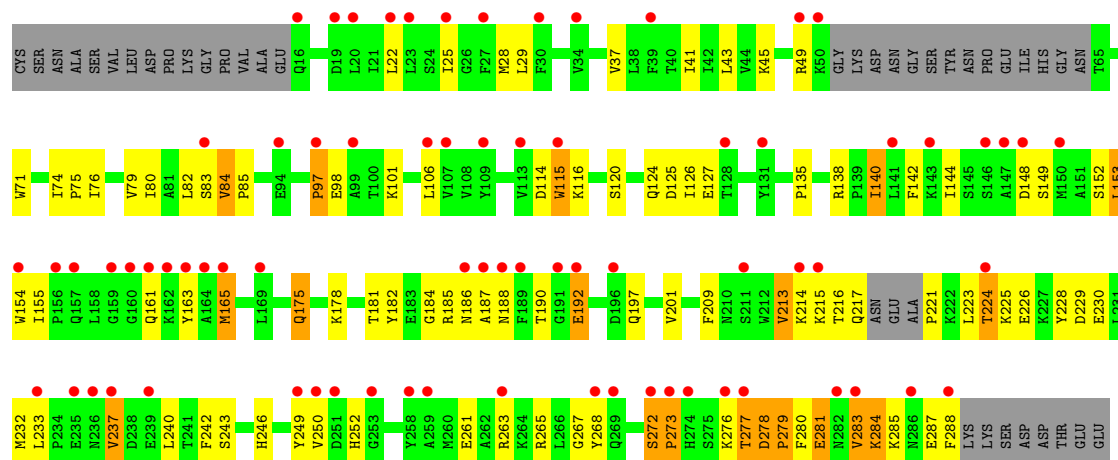
• Molecule 1: AA3-600 quinol oxidase subunit I



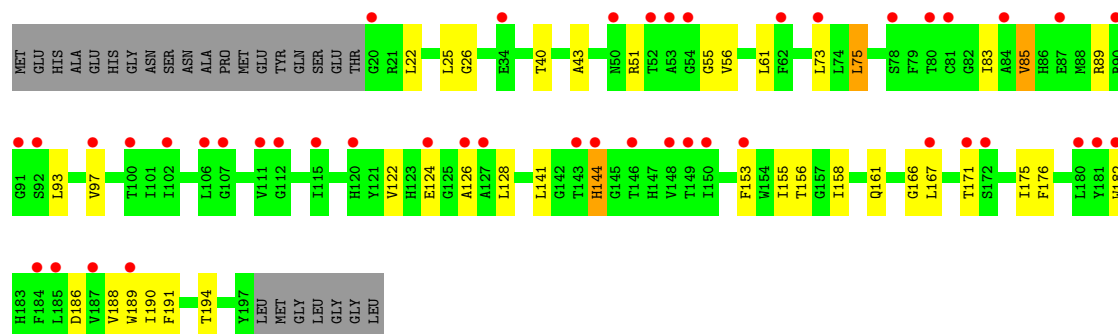




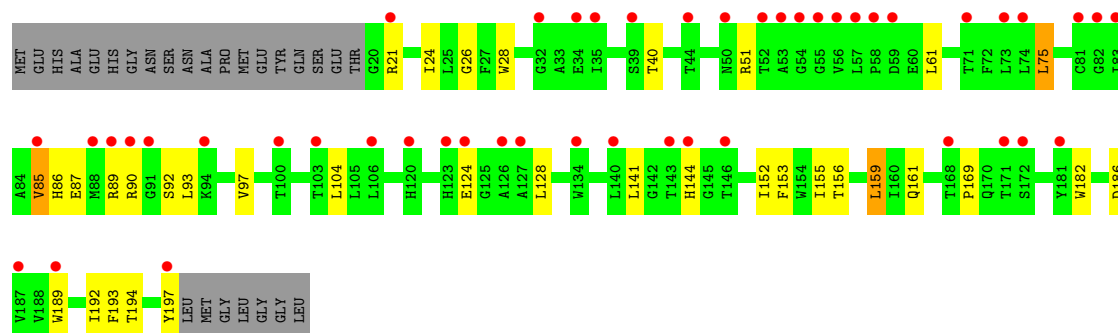
• Molecule 2: Quinol oxidase subunit 2



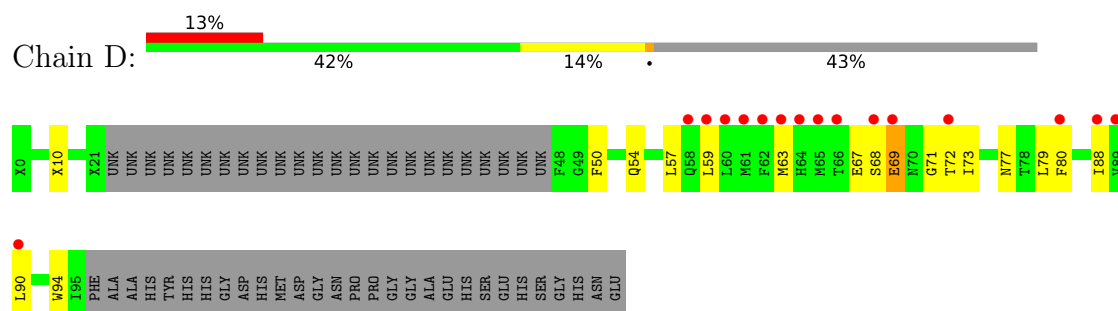
• Molecule 3: AA3-600 quinol oxidase subunit IIII



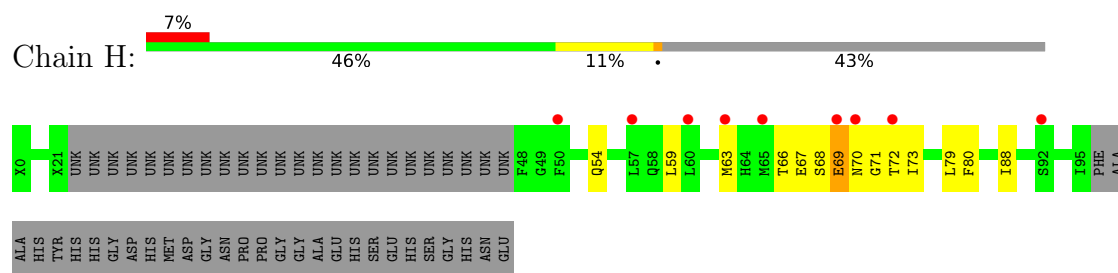
• Molecule 3: AA3-600 quinol oxidase subunit IIII



- 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, α , β , γ	113.93Å 162.20Å 151.32Å 90.00° 109.76° 90.00°	Depositor
Resolution (Å)	48.27 – 3.80 48.27 – 3.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.27-3.80) 98.0 (48.27-3.80)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.14_3235	Depositor
R, R_{free}	0.325 , 0.369 0.328 , 0.370	Depositor DCC
R_{free} test set	2015 reflections (3.94%)	wwPDB-VP
Wilson B-factor (Å ²)	100.9	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 30.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.068 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	17912	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CU, IHQ, 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	0.12	0/5022	0.32	0/6827
1	E	0.11	0/5022	0.31	0/6827
2	B	0.24	0/2122	0.59	0/2879
2	F	0.17	0/2122	0.44	0/2879
3	C	0.09	0/1452	0.26	0/1974
3	G	0.08	0/1452	0.26	0/1974
4	D	0.09	0/381	0.24	0/514
4	H	0.09	0/381	0.25	0/514
All	All	0.14	0/17954	0.37	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 ⓘ

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	155	0
1	E	4855	0	4855	139	0
2	B	2073	0	2061	113	0
2	F	2073	0	2061	67	0
3	C	1411	0	1444	29	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	11	0
5	E	120	0	107	9	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
7	A	14	0	0	1	0
7	E	14	0	0	1	0
All	All	17912	0	17723	497	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 14.

All (497) 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:349:MET:HE1	1:A:395:VAL:HG23	1.63	0.81
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:E:349:MET:HE1	1:E:395:VAL:HG23	1.65	0.77
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:ILE:HG21	1:E:190:LEU:HD22	1.68	0.75
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
1:A:269:MET:HB3	2:B:165:MET:HE1	1.70	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: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:B:230:GLU:O	2:B:284:LYS:NZ	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:121:VAL:HG13	1:E:438:LYS:HZ2	1.65	0.61
2:B:175:GLN:HE21	2:B:176:ALA:C	2.09	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:E:77:MET:HE1	7:E:1004:IHQ:I20	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:414:SER:OG	1:E:464:PHE:O	2.21	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
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
1:A:425:VAL:HG21	5:A:1001:HEA:HMC3	1.87	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
1:E:298:ILE:HD11	1:E:366:MET:HE2	1.87	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:B:250:VAL:C	2:B:252:HIS:H	2.16	0.54
1:A:121:VAL:HG13	1:A:438:LYS:HZ3	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:E:53:HIS:HD2	1:E:131:ASP:HA	1.72	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:188:ASN:HD22	2:B:188:ASN:C	2.17	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:E:361:ASN:O	1:E:365:THR:OG1	2.24	0.52
1:A:140:LEU:O	1:A:144:THR:OG1	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:133:ALA:HA	1:E:211:MET:HE1	1.92	0.51
1:A:126:GLN:HA	1:A:535:LEU:HB2	1.93	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
1:A:77:MET:HE1	7:A:1004:IHQ:I20	2.81	0.50
1:A:392:VAL:HB	2:B:29:LEU:HB3	1.92	0.50
1:E:607:TRP:CD1	1:E:612:VAL:H	2.29	0.50
1:E:54:LYS:NZ	1:E:544:PRO:HB2	2.27	0.50
1:E:298:ILE:HD12	1:E:377:MET:HE1	1.93	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
2:F:250:VAL:C	2:F:252:HIS:H	2.20	0.50
1:E:588:ARG:HE	1:E:624:LEU:HB3	1.77	0.50
1:E:416:PHE:CZ	5:E:1001:HEA:HHD	2.47	0.50
1:A:329:HIS:C	1:A:329:HIS:CD2	2.90	0.49
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
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
1:A:331:PHE:C	1:A:333:THR:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:114:ASP:C	2:B:116:LYS:H	2.20	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:223:MET:HE3	1:A:312:MET:HE2	1.96	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
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
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:145:SER:C	2:B:164:ALA:HB1	2.38	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:141:SER:OG	1:A:200:THR:OG1	2.29	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
1:E:349:MET:HE3	1:E:398:ALA:HB3	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:349:MET:HE3	1:A:398:ALA:HB3	1.98	0.46
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
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:B:165:MET:HB3	2:B:165:MET:HE3	1.72	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:A:298:ILE:HD11	1:A:366:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:VAL:O	1:A:626:SER:OG	2.33	0.45
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:B:124:GLN:CD	2:B:217:GLN:HE21	2.25	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
1:E:235:ILE:HG12	1:E:285:ILE:HD13	1.98	0.45
2:B:233:LEU:HD13	2:B:284:LYS:HZ3	1.82	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
1:A:56:LEU:HA	1:A:59:MET:HE2	1.99	0.44
3:G:155:ILE:O	3:G:159:LEU:HD23	2.18	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:VAL:HA	1:A:247:ALA:HB3	1.99	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:607:TRP:CD1	1:A:612:VAL:H	2.36	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:272:SER:OG	2:B:273:PRO:HD3	2.18	0.43
3:C:55:GLY:C	2:F:225:LYS:HE3	2.43	0.43
1:E:79:ARG:NH2	1:E:467:GLN:OE1	2.36	0.43
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:212:TRP:O	2:B:213:VAL:C	2.62	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
2:B:100:THR:OG1	2:B:104:GLU:OE1	2.37	0.42
2:B:167:GLY:N	2:B:256:ALA:HB2	2.35	0.42
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
1:A:367:TYR:C	1:A:369:GLY:H	2.26	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
2:F:114:ASP:C	2:F:116:LYS:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:MET:HE3	1:E:312:MET:HE2	2.02	0.41
1:E:344:PHE:O	1:E:348:THR:OG1	2.25	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
2:B:127:GLU:CD	2:B:246:HIS:HB3	2.44	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:54:LYS:HZ1	1:E:544:PRO:HB2	1.85	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:125:ASP:C	2:B:126:ILE:HG13	2.46	0.40
4:D:67:GLU:HA	4:D:68:SER:HA	1.66	0.40
2:F:233:LEU:HD13	2:F:284:LYS:HZ3	1.85	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
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:E:367:TYR:C	1:E:369:GLY:H	2.29	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
2:F:165:MET:HE2	2:F:165:MET:HB3	1.89	0.40
2:F:228:TYR:CE1	2:F:232:MET:HE1	2.57	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	603/649 (93%)	510 (85%)	77 (13%)	16 (3%)	4	27
1	E	603/649 (93%)	512 (85%)	77 (13%)	14 (2%)	5	30
2	B	250/296 (84%)	194 (78%)	44 (18%)	12 (5%)	2	17
2	F	250/296 (84%)	195 (78%)	42 (17%)	13 (5%)	1	17
3	C	176/204 (86%)	158 (90%)	17 (10%)	1 (1%)	21	54
3	G	176/204 (86%)	157 (89%)	18 (10%)	1 (1%)	21	54
4	D	46/123 (37%)	39 (85%)	5 (11%)	2 (4%)	2	19
4	H	46/123 (37%)	39 (85%)	5 (11%)	2 (4%)	2	19
All	All	2150/2544 (84%)	1804 (84%)	285 (13%)	61 (3%)	4	26

All (61) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
2	F	278	ASP
1	A	326	VAL

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	512/552 (93%)	485 (95%)	27 (5%)	20	45
1	E	512/552 (93%)	486 (95%)	26 (5%)	21	46
2	B	230/263 (88%)	199 (86%)	31 (14%)	4	19
2	F	230/263 (88%)	210 (91%)	20 (9%)	9	33
3	C	151/171 (88%)	143 (95%)	8 (5%)	20	45
3	G	151/171 (88%)	143 (95%)	8 (5%)	20	45
4	D	38/59 (64%)	36 (95%)	2 (5%)	20	45
4	H	38/59 (64%)	36 (95%)	2 (5%)	20	45
All	All	1862/2090 (89%)	1738 (93%)	124 (7%)	15	41

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	TYR
1	A	79	ARG
1	A	105	ILE
1	A	115	LEU
1	A	145	PHE
1	A	151	LEU
1	A	166	TRP
1	A	172	LEU
1	A	175	ASN
1	A	208	ILE
1	A	209	LEU
1	A	216	MET
1	A	260	PHE

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Mol	Chain	Res	Type
1	A	283	VAL
1	A	288	LEU
1	A	328	THR
1	A	329	HIS
1	A	340	VAL
1	A	349	MET
1	A	363	LEU
1	A	395	VAL
1	A	415	HIS
1	A	416	PHE
1	A	500	PHE
1	A	509	LEU
1	A	552	LEU
1	A	581	HIS
2	B	20	LEU
2	B	29	LEU
2	B	98	GLU
2	B	101	LYS
2	B	103	LYS
2	B	115	TRP
2	B	129	VAL
2	B	134	ILE
2	B	140	ILE
2	B	148	ASP
2	B	153	LEU
2	B	161	GLN
2	B	169	LEU
2	B	171	ASP
2	B	174	LEU
2	B	175	GLN
2	B	188	ASN
2	B	193	HIS
2	B	200	ASP
2	B	201	VAL
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	237	VAL
2	B	252	HIS

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Mol	Chain	Res	Type
2	B	272	SER
2	B	277	THR
2	B	284	LYS
3	C	25	LEU
3	C	56	VAL
3	C	61	LEU
3	C	75	LEU
3	C	85	VAL
3	C	97	VAL
3	C	128	LEU
3	C	144	HIS
4	D	69	GLU
4	D	79	LEU
3	G	61	LEU
3	G	75	LEU
3	G	85	VAL
3	G	97	VAL
3	G	128	LEU
3	G	159	LEU
3	G	161	GLN
3	G	192	ILE
4	H	69	GLU
4	H	79	LEU
2	F	22	LEU
2	F	28	MET
2	F	29	LEU
2	F	115	TRP
2	F	140	ILE
2	F	153	LEU
2	F	165	MET
2	F	175	GLN
2	F	181	THR
2	F	188	ASN
2	F	213	VAL
2	F	215	LYS
2	F	223	LEU
2	F	224	THR
2	F	237	VAL
2	F	246	HIS
2	F	272	SER
2	F	277	THR
2	F	283	VAL

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Mol	Chain	Res	Type
2	F	284	LYS
1	E	36	TYR
1	E	79	ARG
1	E	105	ILE
1	E	115	LEU
1	E	145	PHE
1	E	151	LEU
1	E	166	TRP
1	E	172	LEU
1	E	208	ILE
1	E	209	LEU
1	E	216	MET
1	E	239	PHE
1	E	260	PHE
1	E	283	VAL
1	E	288	LEU
1	E	328	THR
1	E	340	VAL
1	E	349	MET
1	E	363	LEU
1	E	395	VAL
1	E	415	HIS
1	E	416	PHE
1	E	500	PHE
1	E	509	LEU
1	E	552	LEU
1	E	581	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	329	HIS
2	B	188	ASN
2	B	193	HIS
2	B	217	GLN
2	B	236	ASN
2	B	246	HIS
2	B	252	HIS
1	E	20	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	1001	1	67,67,67	2.55	29 (43%)	81,103,103	2.47	31 (38%)
5	HEA	E	1002	-	67,67,67	2.47	26 (38%)	81,103,103	2.60	34 (41%)
7	IHQ	A	1004	-	13,15,21	2.23	3 (23%)	12,22,28	1.40	3 (25%)
5	HEA	A	1002	-	67,67,67	2.46	27 (40%)	81,103,103	2.63	32 (39%)
7	IHQ	E	1004	-	13,15,21	2.17	3 (23%)	12,22,28	1.53	3 (25%)
5	HEA	A	1001	1	67,67,67	2.55	29 (43%)	81,103,103	2.45	31 (38%)

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	1001	1	-	9/36/76/76	-
5	HEA	E	1002	-	-	7/36/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	IHQ	A	1004	-	-	-	0/2/2/2
5	HEA	A	1002	-	-	8/36/76/76	-
7	IHQ	E	1004	-	-	-	0/2/2/2
5	HEA	A	1001	1	-	9/36/76/76	-

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1001	HEA	C3B-C2B	5.76	1.47	1.34
5	A	1001	HEA	C3B-C2B	5.66	1.47	1.34
5	A	1002	HEA	FE-ND	5.64	2.12	1.94
5	E	1002	HEA	FE-ND	5.64	2.12	1.94
5	E	1002	HEA	FE-NB	5.63	2.12	1.94
5	A	1002	HEA	FE-NB	5.53	2.11	1.94
5	A	1002	HEA	C3B-C2B	5.49	1.47	1.34
5	E	1002	HEA	C3B-C2B	5.48	1.47	1.34
7	A	1004	IHQ	C6-C5	5.37	1.49	1.41
7	E	1004	IHQ	C6-C5	5.33	1.49	1.41
5	E	1001	HEA	FE-ND	5.25	2.11	1.94
5	A	1001	HEA	FE-ND	5.24	2.11	1.94
5	A	1001	HEA	C3D-C2D	5.18	1.47	1.36
5	E	1001	HEA	C3D-C2D	5.10	1.47	1.36
5	A	1001	HEA	FE-NB	5.09	2.10	1.94
5	E	1001	HEA	FE-NB	5.06	2.10	1.94
5	A	1001	HEA	C3A-C2A	5.02	1.48	1.37
5	A	1002	HEA	FE-NC	5.02	2.11	1.95
5	E	1001	HEA	C3A-C2A	4.99	1.48	1.37
5	E	1002	HEA	FE-NC	4.98	2.11	1.95
5	E	1002	HEA	C3D-C2D	4.97	1.47	1.36
5	A	1002	HEA	C3D-C2D	4.94	1.47	1.36
5	A	1001	HEA	CHD-C1D	4.91	1.48	1.38
5	A	1001	HEA	CHB-C4A	4.85	1.47	1.38
5	E	1001	HEA	CHD-C1D	4.83	1.48	1.38
5	E	1001	HEA	CHB-C4A	4.81	1.47	1.38
5	E	1001	HEA	CHC-C4B	4.79	1.48	1.38
5	A	1001	HEA	CHC-C4B	4.78	1.48	1.38
5	E	1002	HEA	C3A-C2A	4.74	1.48	1.37
5	A	1002	HEA	C3A-C2A	4.73	1.48	1.37
5	A	1001	HEA	CHA-C1A	4.63	1.47	1.38
5	E	1001	HEA	FE-NC	4.61	2.10	1.95
5	E	1001	HEA	CHA-C1A	4.57	1.47	1.38
5	A	1001	HEA	FE-NC	4.57	2.10	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1002	HEA	CHC-C4B	4.42	1.47	1.38
5	E	1002	HEA	CHC-C4B	4.37	1.47	1.38
5	E	1002	HEA	CHD-C1D	4.35	1.47	1.38
5	E	1002	HEA	CHB-C4A	4.35	1.46	1.38
5	A	1002	HEA	CHD-C1D	4.33	1.47	1.38
7	A	1004	IHQ	C9-N10	4.33	1.41	1.36
5	A	1002	HEA	CHB-C4A	4.23	1.46	1.38
5	A	1002	HEA	CHA-C1A	4.19	1.46	1.38
5	E	1002	HEA	CHA-C1A	4.18	1.46	1.38
7	E	1004	IHQ	C9-N10	4.10	1.41	1.36
5	E	1002	HEA	C1A-NA	4.08	1.47	1.39
5	A	1002	HEA	C1A-NA	4.05	1.47	1.39
5	A	1002	HEA	C4A-NA	3.98	1.47	1.39
5	E	1002	HEA	C4A-NA	3.93	1.47	1.39
5	E	1001	HEA	CHC-C1C	3.87	1.48	1.39
5	A	1001	HEA	CHD-C4C	3.84	1.48	1.39
5	E	1001	HEA	CHD-C4C	3.84	1.48	1.39
5	A	1001	HEA	CHC-C1C	3.81	1.48	1.39
5	E	1001	HEA	CHB-C1B	3.81	1.47	1.39
5	E	1001	HEA	C4A-NA	3.78	1.46	1.39
5	E	1001	HEA	C1A-NA	3.77	1.46	1.39
5	A	1001	HEA	CHB-C1B	3.77	1.47	1.39
5	A	1001	HEA	C1A-NA	3.75	1.46	1.39
5	A	1001	HEA	C4A-NA	3.74	1.46	1.39
5	E	1002	HEA	CHC-C1C	3.49	1.47	1.39
5	E	1002	HEA	CHD-C4C	3.49	1.47	1.39
5	A	1001	HEA	CHA-C4D	3.49	1.47	1.39
5	A	1002	HEA	CHD-C4C	3.43	1.47	1.39
5	E	1001	HEA	CHA-C4D	3.43	1.47	1.39
5	A	1002	HEA	CHC-C1C	3.42	1.47	1.39
7	A	1004	IHQ	O11-N10	3.32	1.44	1.39
5	A	1002	HEA	CHB-C1B	3.28	1.46	1.39
7	E	1004	IHQ	O11-N10	3.26	1.43	1.39
5	E	1002	HEA	CHB-C1B	3.24	1.46	1.39
5	E	1002	HEA	CHA-C4D	3.13	1.46	1.39
5	A	1002	HEA	CHA-C4D	3.05	1.46	1.39
5	E	1001	HEA	C1D-ND	-2.90	1.35	1.40
5	A	1001	HEA	C1D-ND	-2.86	1.35	1.40
5	E	1001	HEA	C4B-NB	-2.85	1.35	1.40
5	A	1001	HEA	C4B-NB	-2.84	1.35	1.40
5	A	1001	HEA	C4B-C3B	2.67	1.49	1.44
5	E	1001	HEA	C1A-C2A	2.66	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1002	HEA	C1D-ND	-2.66	1.35	1.40
5	A	1002	HEA	C1D-ND	-2.66	1.35	1.40
5	E	1001	HEA	C1C-C2C	2.66	1.49	1.43
5	E	1002	HEA	C4B-NB	-2.66	1.35	1.40
5	E	1001	HEA	C4B-C3B	2.64	1.49	1.44
5	A	1002	HEA	C4B-NB	-2.62	1.35	1.40
5	A	1001	HEA	C1A-C2A	2.59	1.49	1.45
5	A	1002	HEA	C1C-C2C	2.57	1.49	1.43
5	A	1001	HEA	C1C-C2C	2.56	1.49	1.43
5	E	1002	HEA	C1C-C2C	2.56	1.49	1.43
5	E	1002	HEA	C4B-C3B	2.55	1.49	1.44
5	A	1002	HEA	C1A-C2A	2.53	1.49	1.45
5	A	1002	HEA	C11-C3B	-2.52	1.48	1.51
5	E	1002	HEA	C11-C3B	-2.51	1.48	1.51
5	A	1002	HEA	C4B-C3B	2.49	1.49	1.44
5	E	1001	HEA	C1D-C2D	2.44	1.49	1.44
5	E	1002	HEA	C1A-C2A	2.40	1.49	1.45
5	E	1001	HEA	C4C-NC	-2.40	1.35	1.39
5	A	1001	HEA	C4C-NC	-2.37	1.35	1.39
5	E	1002	HEA	C1D-C2D	2.35	1.49	1.44
5	A	1001	HEA	C11-C3B	-2.34	1.48	1.51
5	A	1001	HEA	C4D-C3D	2.34	1.49	1.45
5	E	1002	HEA	C4D-C3D	2.34	1.49	1.45
5	A	1001	HEA	C1D-C2D	2.33	1.49	1.44
5	A	1002	HEA	C4D-C3D	2.28	1.48	1.45
5	E	1001	HEA	C4D-C3D	2.28	1.48	1.45
5	A	1002	HEA	C1D-C2D	2.24	1.49	1.44
5	E	1002	HEA	C1B-C2B	2.22	1.49	1.44
5	E	1001	HEA	C11-C3B	-2.19	1.48	1.51
5	A	1001	HEA	C1B-C2B	2.15	1.48	1.44
5	E	1002	HEA	C4C-NC	-2.13	1.35	1.39
5	E	1001	HEA	C1B-C2B	2.13	1.48	1.44
5	A	1002	HEA	C1B-C2B	2.12	1.48	1.44
5	A	1001	HEA	C1C-NC	-2.10	1.35	1.39
5	A	1002	HEA	C4C-NC	-2.09	1.35	1.39
5	A	1001	HEA	C4D-ND	-2.08	1.34	1.38
5	E	1001	HEA	C3C-C4C	2.07	1.48	1.42
5	E	1001	HEA	C4D-ND	-2.07	1.34	1.38
5	A	1002	HEA	C4D-ND	-2.05	1.34	1.38
5	A	1001	HEA	C3C-C4C	2.05	1.48	1.42
5	E	1001	HEA	C3C-C2C	2.01	1.47	1.41

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1002	HEA	C3D-C4D-ND	7.17	117.28	110.35
5	E	1002	HEA	C3D-C4D-ND	6.99	117.11	110.35
5	A	1001	HEA	CHA-C4D-ND	-6.18	117.78	124.42
5	E	1001	HEA	CHA-C4D-ND	-6.09	117.87	124.42
5	E	1001	HEA	C3D-C4D-ND	5.94	116.10	110.35
5	E	1002	HEA	C2B-C1B-NB	5.92	116.75	109.90
5	A	1002	HEA	C2B-C1B-NB	5.84	116.66	109.90
5	A	1001	HEA	C3D-C4D-ND	5.81	115.97	110.35
5	A	1002	HEA	C2D-C1D-ND	5.71	116.40	109.84
5	E	1002	HEA	C3C-C2C-C1C	-5.66	100.50	107.17
5	E	1002	HEA	C2D-C1D-ND	5.65	116.33	109.84
5	A	1002	HEA	C3C-C2C-C1C	-5.64	100.52	107.17
5	E	1002	HEA	C2A-C1A-NA	5.63	115.75	110.32
5	E	1002	HEA	C3B-C4B-NB	5.59	116.27	109.84
5	A	1002	HEA	C3C-C4C-NC	5.58	114.50	109.80
5	A	1002	HEA	C2A-C1A-NA	5.57	115.70	110.32
5	E	1001	HEA	CHA-C1A-NA	-5.56	118.40	124.45
5	E	1001	HEA	C3C-C2C-C1C	-5.43	100.77	107.17
5	A	1001	HEA	CHA-C1A-NA	-5.38	118.60	124.45
5	E	1002	HEA	C3C-C4C-NC	5.36	114.31	109.80
5	A	1001	HEA	C3C-C2C-C1C	-5.34	100.88	107.17
5	A	1002	HEA	C3B-C4B-NB	5.31	115.94	109.84
5	A	1001	HEA	C1A-CHA-C4D	-5.02	115.35	126.02
5	E	1001	HEA	C1A-CHA-C4D	-4.89	115.63	126.02
5	E	1001	HEA	C2A-C1A-NA	4.81	114.97	110.32
5	A	1001	HEA	C2A-C1A-NA	4.62	114.78	110.32
5	A	1002	HEA	CHA-C4D-ND	-4.51	119.57	124.42
5	A	1001	HEA	C2D-C1D-ND	4.49	115.00	109.84
5	E	1001	HEA	C2D-C1D-ND	4.44	114.95	109.84
5	A	1001	HEA	C3B-C4B-NB	4.42	114.92	109.84
5	A	1001	HEA	C2B-C1B-NB	4.40	114.99	109.90
5	E	1001	HEA	C3B-C4B-NB	4.40	114.90	109.84
5	E	1001	HEA	C3C-C4C-NC	4.37	113.48	109.80
5	E	1001	HEA	C2B-C1B-NB	4.37	114.95	109.90
5	A	1002	HEA	C2C-C1C-NC	4.25	116.96	110.14
5	A	1002	HEA	C1D-C2D-C3D	-4.25	102.51	106.98
5	E	1002	HEA	C2C-C1C-NC	4.24	116.94	110.14
5	E	1002	HEA	C1D-C2D-C3D	-4.22	102.54	106.98
5	E	1002	HEA	C3A-C2A-C1A	-4.21	103.06	107.05
5	A	1002	HEA	C3A-C2A-C1A	-4.17	103.10	107.05
5	E	1001	HEA	C3A-C2A-C1A	-4.17	103.10	107.05
5	A	1002	HEA	CHA-C1A-NA	-4.16	119.92	124.45
5	A	1001	HEA	C3C-C4C-NC	4.15	113.29	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1002	HEA	CHA-C4D-ND	-4.14	119.96	124.42
5	A	1002	HEA	C1B-C2B-C3B	-4.06	102.10	106.80
5	A	1001	HEA	C3A-C2A-C1A	-4.05	103.21	107.05
5	E	1002	HEA	C1B-C2B-C3B	-4.03	102.13	106.80
5	A	1001	HEA	C1D-C2D-C3D	-3.77	103.01	106.98
5	E	1001	HEA	C1D-C2D-C3D	-3.75	103.04	106.98
5	E	1001	HEA	C2C-C1C-NC	3.59	115.90	110.14
5	A	1001	HEA	C2C-C1C-NC	3.53	115.80	110.14
5	A	1002	HEA	C4D-C3D-C2D	-3.51	101.78	106.89
5	E	1002	HEA	CHA-C1A-NA	-3.46	120.69	124.45
5	E	1002	HEA	C4D-C3D-C2D	-3.44	101.88	106.89
5	A	1002	HEA	C13-C14-C15	-3.40	119.85	127.62
5	E	1001	HEA	C4D-C3D-C2D	-3.34	102.03	106.89
5	A	1001	HEA	C4D-C3D-C2D	-3.32	102.06	106.89
5	A	1002	HEA	C4A-NA-C1A	-3.32	100.41	105.82
5	E	1002	HEA	C4A-NA-C1A	-3.28	100.48	105.82
5	E	1001	HEA	C1B-C2B-C3B	-3.27	103.02	106.80
5	A	1001	HEA	C1B-C2B-C3B	-3.26	103.02	106.80
5	A	1001	HEA	CHB-C1B-NB	-3.24	120.94	124.42
7	E	1004	IHQ	C13-C9-C8	-3.23	118.12	123.77
5	E	1002	HEA	CHB-C1B-NB	-3.22	120.95	124.42
5	E	1001	HEA	C17-C18-C19	-3.14	120.44	127.62
5	E	1002	HEA	C26-C15-C16	3.04	120.50	115.23
5	E	1001	HEA	CHB-C1B-NB	-3.04	121.15	124.42
5	E	1002	HEA	C13-C14-C15	-3.02	120.71	127.62
5	A	1001	HEA	C17-C18-C19	-3.00	120.75	127.62
5	E	1001	HEA	C26-C15-C16	3.00	120.43	115.23
5	A	1002	HEA	C26-C15-C16	2.96	120.37	115.23
7	E	1004	IHQ	C13-C9-N10	2.95	120.73	117.28
5	A	1001	HEA	C26-C15-C16	2.94	120.33	115.23
5	A	1002	HEA	C17-C18-C19	-2.93	120.92	127.62
5	E	1001	HEA	C4B-C3B-C2B	-2.91	102.55	107.44
5	A	1002	HEA	C27-C19-C20	2.90	120.27	115.23
5	E	1002	HEA	C4B-C3B-C2B	-2.89	102.58	107.44
5	A	1001	HEA	C4B-C3B-C2B	-2.88	102.60	107.44
5	E	1002	HEA	C17-C18-C19	-2.84	121.13	127.62
7	A	1004	IHQ	C13-C9-C8	-2.78	118.92	123.77
5	A	1002	HEA	C4B-C3B-C2B	-2.76	102.80	107.44
5	A	1001	HEA	CHC-C4B-NB	-2.75	120.96	124.37
5	A	1002	HEA	CHB-C1B-NB	-2.75	121.47	124.42
5	E	1001	HEA	CHC-C4B-NB	-2.71	121.01	124.37
5	A	1002	HEA	C1D-ND-C4D	-2.69	102.02	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1002	HEA	C13-C12-C11	-2.65	110.16	114.39
5	A	1001	HEA	CAD-C3D-C4D	2.64	129.29	124.70
7	A	1004	IHQ	C13-C9-N10	2.63	120.35	117.28
5	E	1001	HEA	C27-C19-C20	2.61	119.75	115.23
5	E	1001	HEA	CMD-C2D-C1D	2.60	129.10	125.03
5	E	1002	HEA	CMB-C2B-C1B	2.60	129.09	125.03
5	E	1002	HEA	C1D-ND-C4D	-2.59	102.14	105.21
5	E	1001	HEA	CAD-C3D-C4D	2.59	129.20	124.70
5	E	1002	HEA	CHC-C1C-C2C	-2.59	119.92	127.43
5	E	1002	HEA	C27-C19-C20	2.54	119.64	115.23
5	A	1002	HEA	CHC-C1C-C2C	-2.52	120.11	127.43
5	E	1001	HEA	CHB-C4A-NA	-2.52	121.71	124.45
5	E	1002	HEA	C4B-NB-C1B	-2.48	102.27	105.21
5	A	1001	HEA	CMB-C2B-C1B	2.48	128.91	125.03
5	A	1002	HEA	CMB-C2B-C1B	2.47	128.90	125.03
5	A	1001	HEA	C27-C19-C20	2.45	119.49	115.23
5	E	1001	HEA	C4A-NA-C1A	-2.43	101.85	105.82
5	A	1002	HEA	C25-C23-C24	2.38	120.06	114.59
5	A	1001	HEA	CMD-C2D-C1D	2.37	128.73	125.03
5	E	1002	HEA	CAD-C3D-C4D	2.36	128.82	124.70
5	A	1001	HEA	C13-C14-C15	-2.36	122.23	127.62
5	A	1001	HEA	CHB-C4A-NA	-2.35	121.90	124.45
5	E	1001	HEA	C25-C23-C24	2.32	119.93	114.59
5	A	1001	HEA	C4A-NA-C1A	-2.32	102.04	105.82
5	E	1002	HEA	C25-C23-C24	2.31	119.91	114.59
5	E	1002	HEA	CHB-C4A-NA	-2.29	121.96	124.45
5	E	1001	HEA	CMB-C2B-C1B	2.29	128.61	125.03
5	A	1002	HEA	C4B-NB-C1B	-2.29	102.50	105.21
5	E	1002	HEA	CMD-C2D-C1D	2.26	128.57	125.03
5	A	1002	HEA	CAD-C3D-C4D	2.24	128.60	124.70
5	A	1001	HEA	OMA-CMA-C3A	-2.21	120.63	125.62
5	A	1001	HEA	C25-C23-C24	2.21	119.68	114.59
5	E	1002	HEA	C1A-CHA-C4D	-2.21	121.33	126.02
7	A	1004	IHQ	C5-C6-C7	-2.21	119.28	121.38
5	E	1001	HEA	C13-C14-C15	-2.20	122.59	127.62
5	E	1001	HEA	CHD-C1D-ND	-2.19	121.66	124.37
5	A	1002	HEA	CHD-C1D-C2D	-2.15	120.83	126.95
5	E	1002	HEA	CHD-C1D-C2D	-2.12	120.91	126.95
5	A	1002	HEA	CMD-C2D-C1D	2.11	128.33	125.03
7	E	1004	IHQ	C5-C6-C7	-2.10	119.38	121.38
5	A	1002	HEA	CHB-C4A-NA	-2.06	122.21	124.45
5	E	1002	HEA	C13-C12-C11	-2.05	111.12	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	HEA	CMC-C2C-C3C	2.04	131.35	126.55
5	A	1001	HEA	CHD-C1D-ND	-2.04	121.85	124.37
5	E	1001	HEA	OMA-CMA-C3A	-2.03	121.03	125.62
5	E	1001	HEA	C21-C22-C23	-2.02	120.91	127.64
5	A	1002	HEA	C21-C22-C23	-2.02	120.92	127.64
5	E	1002	HEA	C21-C22-C23	-2.02	120.92	127.64
5	E	1002	HEA	CMC-C2C-C1C	2.01	128.48	125.42

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	HEA	C2A-C3A-CMA-OMA
5	A	1001	HEA	C4A-C3A-CMA-OMA
5	A	1001	HEA	C3B-C11-C12-C13
5	A	1001	HEA	O11-C11-C12-C13
5	E	1001	HEA	C2A-C3A-CMA-OMA
5	E	1001	HEA	C4A-C3A-CMA-OMA
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	E	1002	HEA	CAD-CBD-CGD-O2D
5	A	1002	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	C2D-C3D-CAD-CBD
5	E	1002	HEA	C2D-C3D-CAD-CBD
5	A	1001	HEA	CAD-CBD-CGD-O2D
5	E	1001	HEA	CAD-CBD-CGD-O2D
5	A	1002	HEA	C4D-C3D-CAD-CBD
5	A	1002	HEA	CAA-CBA-CGA-O2A
5	E	1002	HEA	CAA-CBA-CGA-O2A
5	A	1002	HEA	C2A-C3A-CMA-OMA
5	E	1002	HEA	CAA-CBA-CGA-O1A
5	A	1002	HEA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
5	A	1001	HEA	CAD-CBD-CGD-O1D
5	E	1001	HEA	CAD-CBD-CGD-O1D
5	E	1002	HEA	C4D-C3D-CAD-CBD

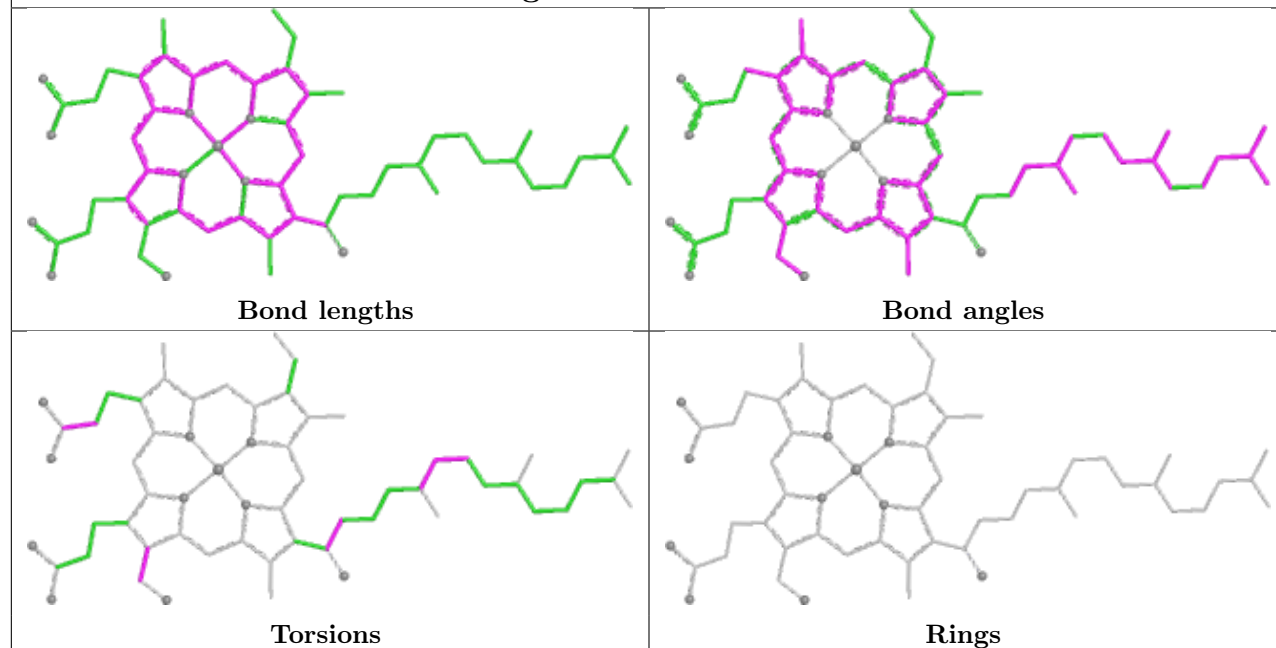
There are no ring outliers.

6 monomers are involved in 22 short contacts:

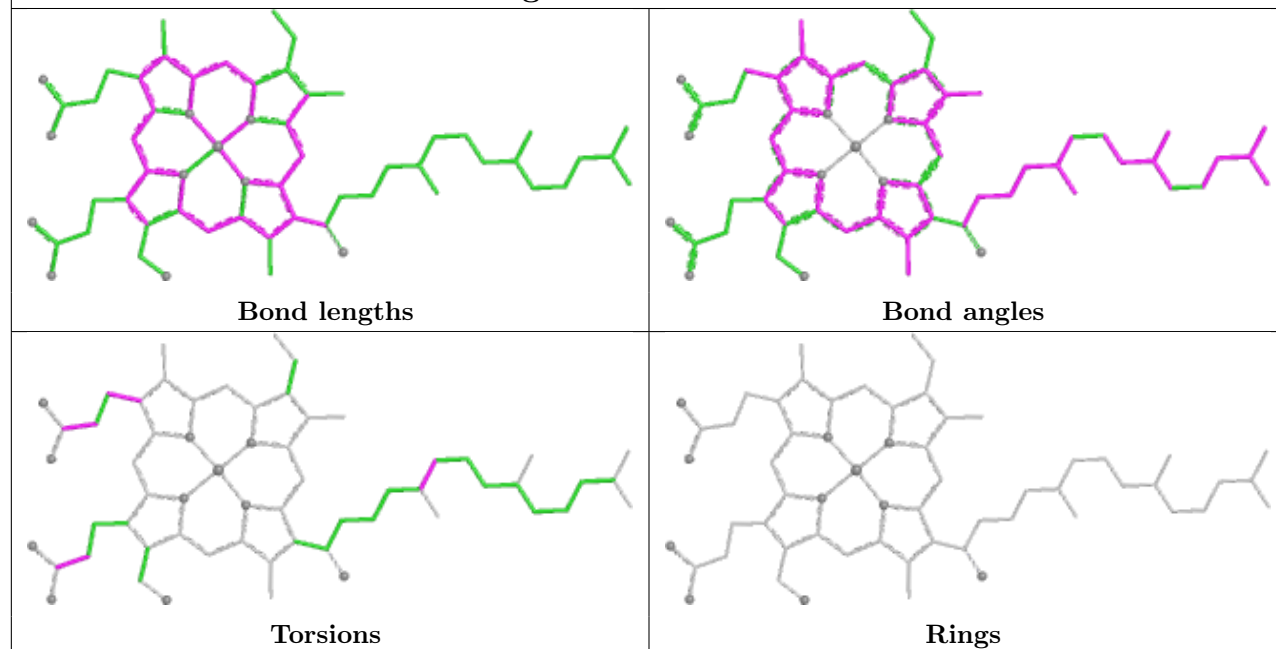
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1001	HEA	4	0
5	E	1002	HEA	5	0
7	A	1004	IHQ	1	0
5	A	1002	HEA	5	0
7	E	1004	IHQ	1	0
5	A	1001	HEA	6	0

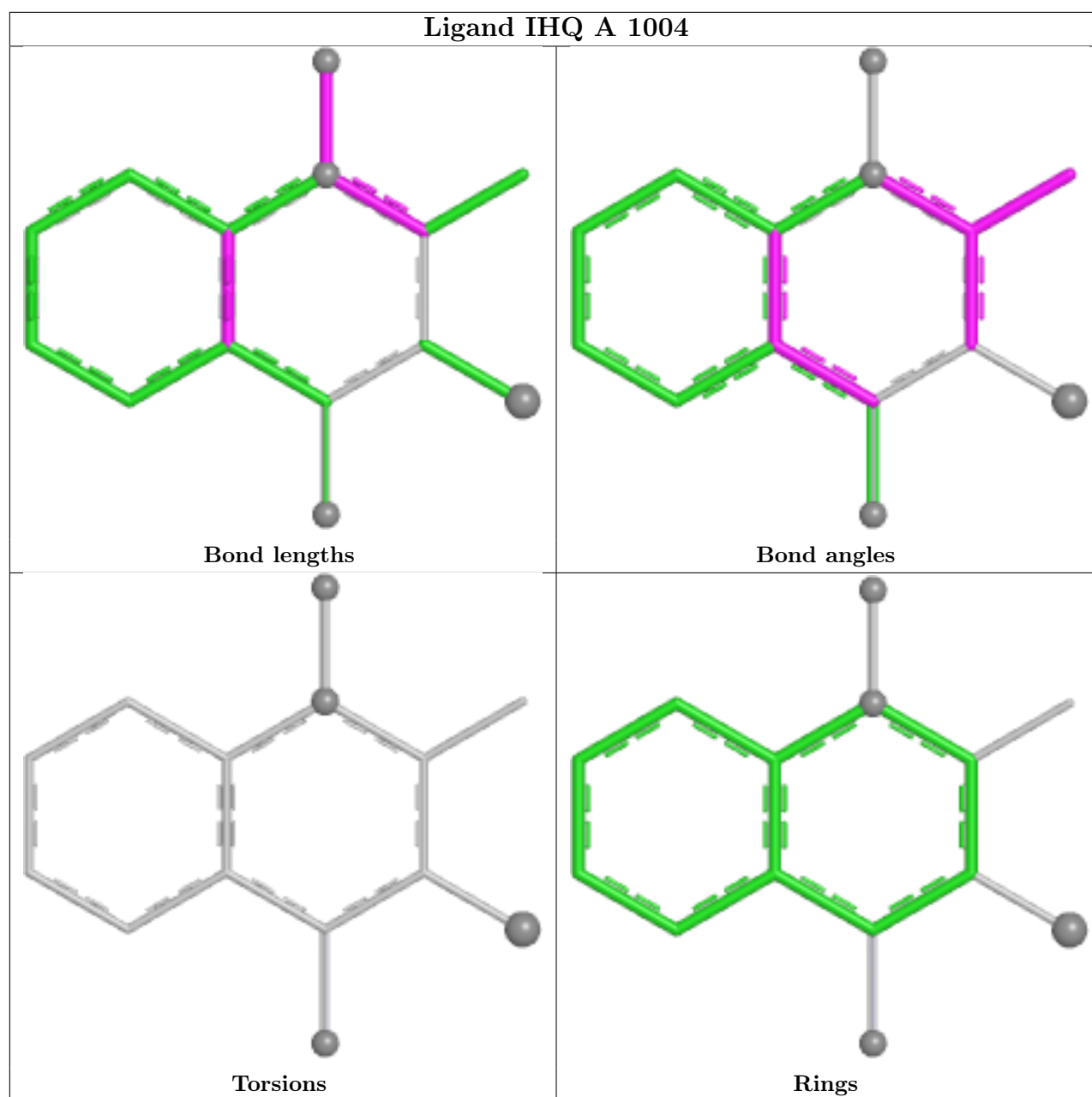
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

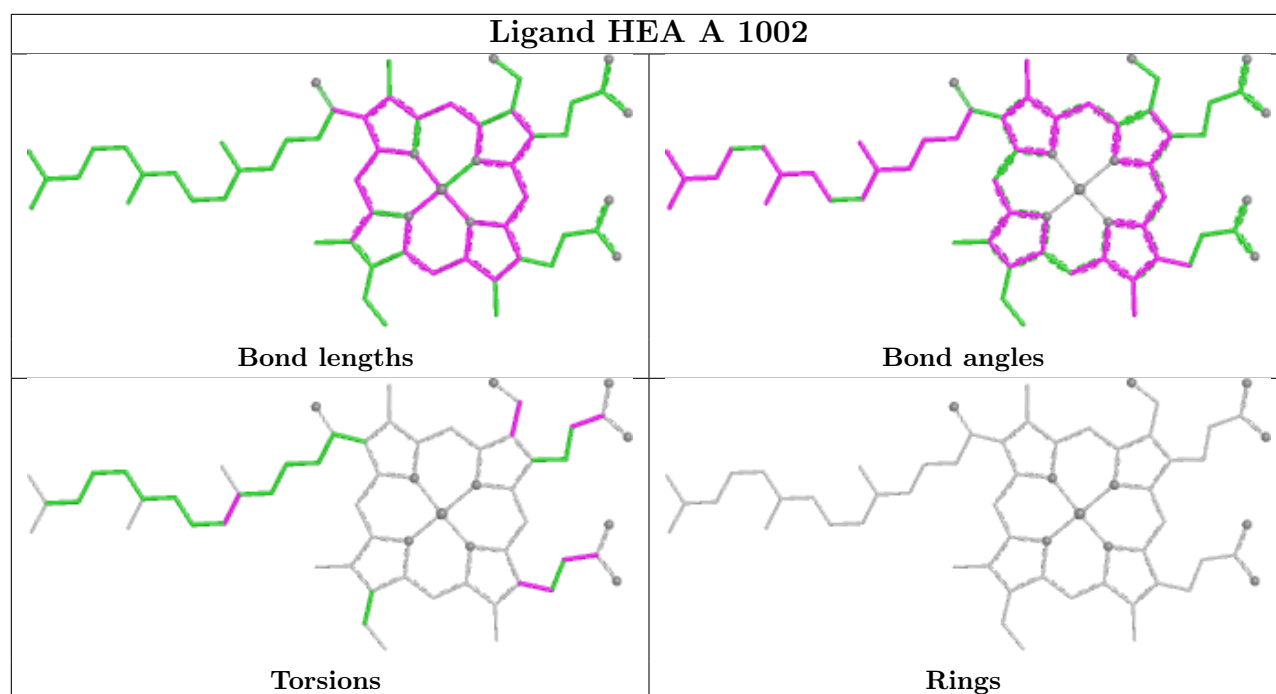
Ligand HEA E 1001

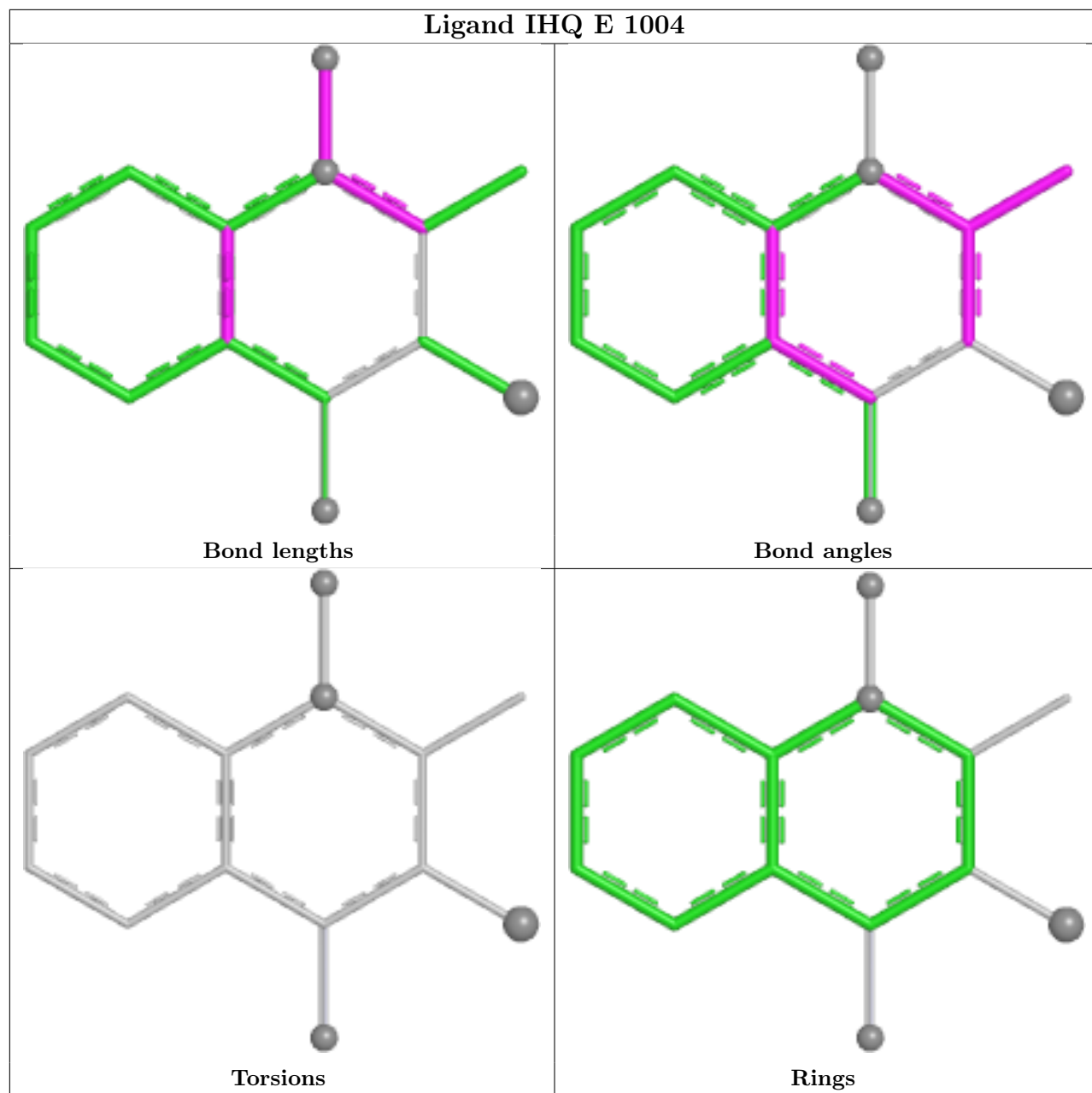


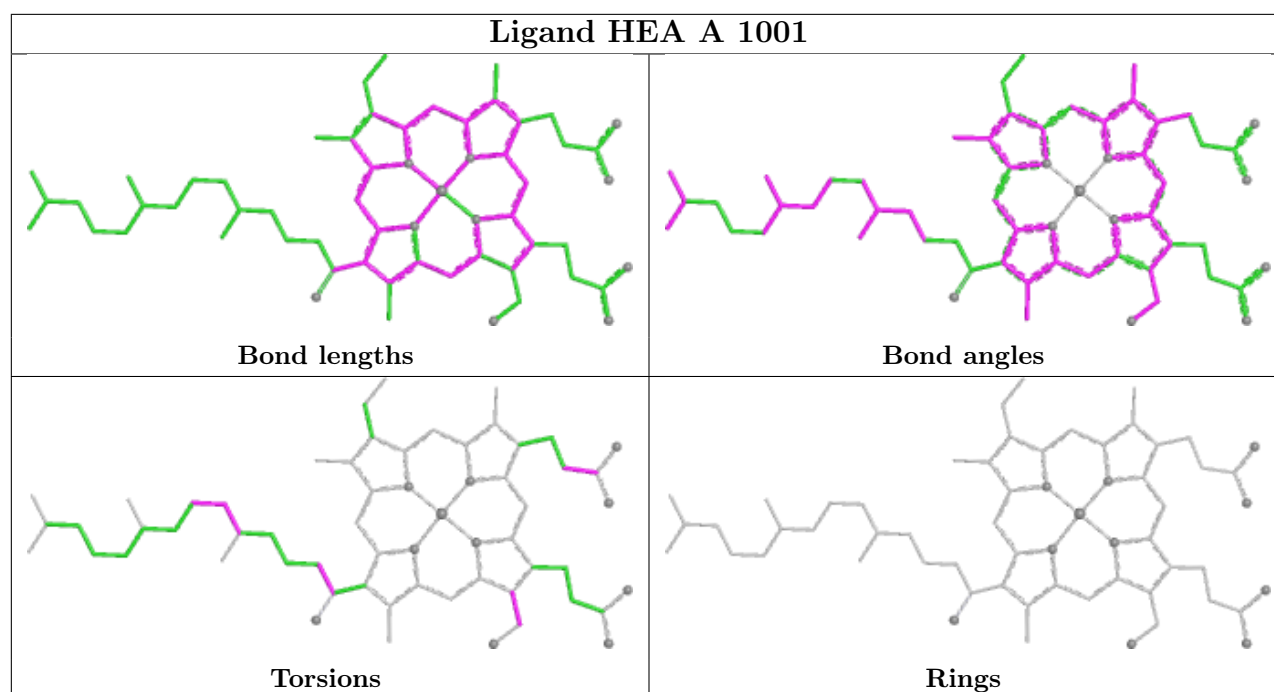
Ligand HEA E 1002











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	607/649 (93%)	1.62	185 (30%)  	52, 115, 170, 235	0
1	E	607/649 (93%)	1.70	190 (31%)  	58, 117, 182, 232	0
2	B	256/296 (86%)	1.73	76 (29%)  	71, 145, 209, 264	0
2	F	256/296 (86%)	1.50	74 (28%)  	57, 142, 206, 254	0
3	C	178/204 (87%)	1.37	45 (25%)  	69, 122, 185, 208	0
3	G	178/204 (87%)	1.54	47 (26%)  	65, 125, 196, 241	0
4	D	48/123 (39%)	1.67	16 (33%)  	73, 118, 172, 196	0
4	H	48/123 (39%)	1.20	9 (18%)  	76, 117, 172, 180	0
All	All	2178/2544 (85%)	1.60	642 (29%)  	52, 123, 190, 264	0

All (642) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	333	THR	14.5
2	B	97	PRO	12.1
4	D	69	GLU	11.4
2	B	98	GLU	11.1
2	B	16	GLN	9.6
2	B	73	VAL	9.5
2	B	92	SER	9.5
1	E	407	HIS	9.2
2	B	95	LYS	9.1
1	E	334	MET	9.0
1	E	405	GLN	8.9
3	G	124	GLU	8.8
2	F	163	TYR	8.6
2	B	96	ALA	8.5
1	E	580	ILE	8.5
1	A	86	ASN	8.4

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Mol	Chain	Res	Type	RSRZ
1	E	404	TYR	8.2
1	E	332	PHE	8.0
1	E	213	THR	7.9
1	A	437	PRO	7.9
1	E	406	TYR	7.7
1	E	130	ARG	7.7
1	A	432	PHE	7.6
1	A	507	LEU	7.5
1	A	167	THR	7.1
2	B	274	HIS	7.1
1	A	578	LYS	7.0
1	E	128	GLY	7.0
1	E	615	LEU	6.9
1	E	335	GLY	6.8
1	E	211	MET	6.8
4	D	59	LEU	6.8
1	A	510	CYS	6.7
3	G	90	ARG	6.7
3	C	181	TYR	6.7
1	A	469	PHE	6.7
1	E	408	ASN	6.7
1	E	619	LEU	6.7
1	A	314	GLY	6.6
2	B	190	THR	6.6
2	F	214	LYS	6.6
2	F	19	ASP	6.5
1	A	166	TRP	6.5
2	B	187	ALA	6.4
4	D	60	LEU	6.4
1	A	541	SER	6.3
1	E	244	VAL	6.3
1	A	269	MET	6.3
1	E	303	ARG	6.2
3	G	144	HIS	6.2
4	D	63	MET	6.1
1	A	163	ASN	6.0
1	E	584	SER	6.0
3	C	97	VAL	5.9
1	E	305	GLN	5.9
2	B	282	ASN	5.8
1	E	412	LEU	5.8
2	F	215	LYS	5.8

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Mol	Chain	Res	Type	RSRZ
1	E	331	PHE	5.7
1	A	540	SER	5.7
1	E	95	TYR	5.6
1	E	212	ARG	5.6
1	E	445	ASN	5.6
1	A	550	ALA	5.6
1	E	191	GLN	5.5
1	A	543	ILE	5.5
2	B	17	GLN	5.4
2	F	253	GLY	5.4
3	C	107	GLY	5.3
3	G	89	ARG	5.3
1	E	372	SER	5.2
2	B	236	ASN	5.1
1	E	269	MET	5.1
1	E	613	VAL	5.1
1	A	93	ASN	5.0
3	G	126	ALA	4.9
1	A	577	PHE	4.9
1	A	478	ARG	4.9
4	D	58	GLN	4.9
1	E	403	ASP	4.9
2	B	277	THR	4.8
1	A	542	ALA	4.8
2	F	161	GLN	4.8
1	A	408	ASN	4.8
3	C	50	ASN	4.8
3	G	57	LEU	4.8
1	E	210	LYS	4.7
2	B	154	TRP	4.7
1	E	157	VAL	4.7
1	E	370	ARG	4.7
1	E	29	ALA	4.7
3	G	52	THR	4.7
2	B	186	ASN	4.7
3	G	55	GLY	4.7
1	A	491	LEU	4.6
1	A	175	ASN	4.6
2	F	30	PHE	4.6
1	E	587	GLY	4.5
4	H	69	GLU	4.5
1	A	318	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	440	PHE	4.5
2	B	34	VAL	4.4
1	A	622	MET	4.4
3	C	171	THR	4.4
1	E	247	ALA	4.4
2	F	169	LEU	4.4
1	E	468	TYR	4.4
2	B	20	LEU	4.4
2	F	277	THR	4.4
1	E	161	SER	4.4
1	A	296	GLU	4.4
1	A	428	CYS	4.4
4	H	63	MET	4.3
1	A	579	LYS	4.3
1	E	336	ASN	4.3
1	E	33	VAL	4.3
1	A	317	ILE	4.3
1	A	48	ILE	4.3
1	A	54	LYS	4.2
3	G	85	VAL	4.2
1	A	62	ILE	4.2
3	G	140	LEU	4.2
1	A	488	TRP	4.2
1	A	164	ALA	4.1
1	A	477	ARG	4.1
2	F	211	SER	4.1
3	G	39	SER	4.1
3	G	35	ILE	4.1
3	G	21	ARG	4.1
1	A	58	ILE	4.1
1	A	436	TYR	4.1
1	A	388	VAL	4.1
1	A	618	VAL	4.1
4	D	72	THR	4.1
1	A	136	TYR	4.1
2	B	163	TYR	4.1
1	A	385	PRO	4.1
1	A	55	LYS	4.0
2	B	99	ALA	4.0
1	E	537	TRP	4.0
1	E	216	MET	4.0
3	C	187	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
3	C	146	THR	4.0
3	G	171	THR	4.0
2	F	115	TRP	3.9
1	A	61	ILE	3.9
1	A	275	PHE	3.9
1	E	263	GLU	3.9
2	F	236	ASN	3.9
1	A	441	GLY	3.9
3	C	148	VAL	3.9
1	A	307	PHE	3.8
2	B	70	VAL	3.8
1	E	178	SER	3.8
1	E	273	ASN	3.8
1	A	47	TRP	3.8
2	F	99	ALA	3.8
1	A	482	TYR	3.8
1	E	516	SER	3.8
3	C	53	ALA	3.8
1	A	357	VAL	3.8
1	E	350	ALA	3.7
1	A	121	VAL	3.7
1	E	482	TYR	3.7
2	B	259	ALA	3.7
3	G	56	VAL	3.7
2	B	173	TYR	3.7
2	F	165	MET	3.7
1	A	434	PHE	3.7
1	E	392	VAL	3.7
1	A	92	SER	3.6
1	A	358	LYS	3.6
2	F	276	LYS	3.6
1	E	169	TYR	3.6
3	G	32	GLY	3.6
3	C	90	ARG	3.6
2	F	156	PRO	3.6
1	A	267	MET	3.6
1	A	52	ASP	3.6
1	E	32	PHE	3.6
1	A	172	LEU	3.6
3	C	126	ALA	3.6
1	E	224	PHE	3.6
1	E	166	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	582	MET	3.5
1	E	618	VAL	3.5
1	E	330	HIS	3.5
2	F	189	PHE	3.5
1	A	379	TRP	3.5
1	A	392	VAL	3.5
3	C	149	THR	3.5
1	E	175	ASN	3.5
1	E	492	ASN	3.5
1	E	480	TYR	3.5
1	E	616	ILE	3.5
1	E	610	MET	3.5
1	A	263	GLU	3.5
3	C	73	LEU	3.5
1	E	341	ASN	3.5
3	C	106	LEU	3.4
3	C	185	LEU	3.4
1	A	466	PRO	3.4
1	E	448	ILE	3.4
1	A	225	THR	3.4
1	E	327	TRP	3.4
2	B	191	GLY	3.4
2	F	27	PHE	3.4
2	B	189	PHE	3.4
2	F	274	HIS	3.4
1	E	90	LEU	3.4
3	G	50	ASN	3.4
3	G	181	TYR	3.4
1	E	304	LYS	3.4
1	E	393	THR	3.4
1	A	171	PRO	3.4
2	F	282	ASN	3.4
1	E	165	GLY	3.3
1	E	192	ILE	3.3
1	E	606	GLU	3.3
2	B	74	ILE	3.3
1	A	480	TYR	3.3
2	B	150	MET	3.3
2	F	269	GLN	3.3
1	E	609	TRP	3.3
2	F	23	LEU	3.3
3	G	82	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	439	MET	3.3
1	A	371	ILE	3.3
3	G	34	GLU	3.3
1	A	473	GLN	3.3
1	A	455	ILE	3.3
1	A	620	LEU	3.3
2	B	37	VAL	3.3
1	E	455	ILE	3.2
2	B	165	MET	3.2
1	E	214	LYS	3.2
1	A	629	TYR	3.2
1	A	619	LEU	3.2
2	B	258	TYR	3.2
1	A	282	GLU	3.2
1	E	596	PHE	3.2
1	A	609	TRP	3.2
1	A	487	GLY	3.2
1	A	632	GLY	3.2
1	E	96	ASN	3.2
1	A	438	LYS	3.2
1	E	276	TRP	3.2
2	F	154	TRP	3.2
3	G	54	GLY	3.2
1	A	405	GLN	3.2
2	F	34	VAL	3.2
1	A	137	LEU	3.2
2	B	31	ILE	3.2
3	C	189	TRP	3.2
3	G	91	GLY	3.2
2	F	50	LYS	3.2
1	A	222	PRO	3.2
1	A	224	PHE	3.1
3	C	102	ILE	3.1
1	A	492	ASN	3.1
1	A	416	PHE	3.1
2	B	225	LYS	3.1
1	A	633	TYR	3.1
1	A	161	SER	3.1
1	A	486	ASP	3.1
1	E	583	PRO	3.1
1	E	349	MET	3.1
1	A	262	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	197	THR	3.1
2	F	283	VAL	3.1
3	G	53	ALA	3.1
3	C	180	LEU	3.1
3	G	100	THR	3.1
1	E	321	VAL	3.1
1	A	608	TYR	3.1
1	E	542	ALA	3.1
2	F	235	GLU	3.1
1	A	368	LYS	3.1
2	B	269	GLN	3.0
1	A	495	SER	3.0
1	A	114	PHE	3.0
1	A	362	TRP	3.0
1	E	116	ILE	3.0
1	E	115	LEU	3.0
1	A	546	HIS	3.0
2	F	107	VAL	3.0
1	A	445	ASN	3.0
1	E	248	LEU	3.0
2	B	94	GLU	3.0
3	C	34	GLU	3.0
1	A	85	PRO	3.0
1	E	289	PRO	3.0
1	E	76	LEU	3.0
1	E	415	HIS	3.0
2	B	188	ASN	3.0
1	E	78	MET	3.0
1	E	352	SER	2.9
2	B	18	SER	2.9
1	E	585	ASN	2.9
1	E	411	PHE	2.9
1	A	18	GLY	2.9
1	A	305	GLN	2.9
1	A	489	THR	2.9
2	B	161	GLN	2.9
3	C	100	THR	2.9
1	A	238	ALA	2.9
2	F	164	ALA	2.9
3	C	127	ALA	2.9
1	E	568	LYS	2.9
1	A	407	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	563	HIS	2.9
1	E	598	LEU	2.9
1	E	181	PRO	2.9
1	A	349	MET	2.9
1	E	167	THR	2.9
3	G	120	HIS	2.9
1	E	27	THR	2.9
1	A	610	MET	2.9
2	F	150	MET	2.9
1	E	79	ARG	2.9
1	E	94	HIS	2.9
2	B	152	SER	2.9
3	C	92	SER	2.9
1	A	381	LEU	2.9
2	B	91	TYR	2.9
1	A	177	MET	2.8
1	E	465	PHE	2.8
1	A	372	SER	2.8
3	C	78	SER	2.8
3	C	172	SER	2.8
2	B	252	HIS	2.8
3	G	187	VAL	2.8
2	F	268	TYR	2.8
2	B	108	VAL	2.8
2	B	281	GLU	2.8
1	E	164	ALA	2.8
1	A	147	VAL	2.8
1	A	219	MET	2.8
1	A	530	GLY	2.8
3	G	127	ALA	2.8
3	G	172	SER	2.8
2	F	109	TYR	2.8
2	F	106	LEU	2.7
3	C	167	LEU	2.7
1	E	162	PRO	2.7
1	A	356	GLY	2.7
1	E	184	ASN	2.7
2	B	210	ASN	2.7
1	A	327	TRP	2.7
1	A	605	PHE	2.7
1	E	530	GLY	2.7
1	A	243	THR	2.7

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Mol	Chain	Res	Type	RSRZ
3	G	73	LEU	2.7
1	A	512	ASN	2.7
1	A	66	ILE	2.7
1	A	88	SER	2.7
1	E	131	ASP	2.7
1	E	607	TRP	2.7
3	G	94	LYS	2.7
1	A	449	GLY	2.7
1	E	515	TYR	2.7
2	F	191	GLY	2.7
1	A	63	SER	2.7
1	E	240	PRO	2.7
1	E	410	TYR	2.7
2	F	159	GLY	2.7
2	F	94	GLU	2.7
3	C	87	GLU	2.7
1	E	301	PHE	2.7
1	E	549	PHE	2.7
4	D	68	SER	2.7
1	A	176	ASP	2.7
2	B	102	ASP	2.7
1	E	366	MET	2.7
1	E	22	SER	2.7
1	A	268	PRO	2.6
1	E	18	GLY	2.6
1	E	264	ALA	2.6
3	C	143	THR	2.6
1	A	506	PHE	2.6
1	A	627	PHE	2.6
2	B	30	PHE	2.6
2	B	240	LEU	2.6
1	A	621	CYS	2.6
2	B	201	VAL	2.6
2	B	193	HIS	2.6
2	F	160	GLY	2.6
3	C	54	GLY	2.6
3	C	124	GLU	2.6
1	E	605	PHE	2.6
1	E	477	ARG	2.6
3	C	115	ILE	2.6
4	D	64	HIS	2.6
1	A	465	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	83	SER	2.6
1	E	504	VAL	2.6
3	C	144	HIS	2.6
3	G	74	LEU	2.6
1	A	418	TYR	2.6
1	E	608	TYR	2.6
2	B	194	PHE	2.6
3	G	44	THR	2.6
1	A	96	ASN	2.6
1	E	70	ARG	2.6
2	B	50	LYS	2.6
1	E	129	ALA	2.6
1	E	417	HIS	2.6
1	A	134	PHE	2.6
1	E	514	TYR	2.6
2	F	162	LYS	2.6
1	A	306	LEU	2.6
1	E	552	LEU	2.6
1	E	558	GLN	2.6
2	B	279	PRO	2.6
2	F	273	PRO	2.6
1	E	61	ILE	2.5
1	E	293	ILE	2.5
1	E	478	ARG	2.5
2	F	188	ASN	2.5
1	E	290	ALA	2.5
1	E	402	ALA	2.5
2	F	147	ALA	2.5
1	A	355	THR	2.5
1	A	504	VAL	2.5
1	E	612	VAL	2.5
2	B	235	GLU	2.5
1	E	15	LEU	2.5
1	E	562	LEU	2.5
2	F	22	LEU	2.5
1	E	296	GLU	2.5
2	B	90	ILE	2.5
3	C	20	GLY	2.5
3	G	83	ILE	2.5
1	E	209	LEU	2.5
4	H	92	SER	2.5
1	E	574	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	192	GLU	2.5
3	G	88	MET	2.5
1	A	448	ILE	2.5
1	A	508	ILE	2.5
2	B	148	ASP	2.5
3	C	150	ILE	2.5
2	F	249	TYR	2.5
2	F	39	PHE	2.5
1	E	620	LEU	2.5
2	F	83	SER	2.5
1	E	136	TYR	2.5
1	E	485	ASN	2.4
1	A	363	LEU	2.4
1	A	165	GLY	2.4
1	E	369	GLY	2.4
3	C	91	GLY	2.4
2	F	237	VAL	2.4
3	C	111	VAL	2.4
1	A	410	TYR	2.4
1	A	429	PHE	2.4
1	A	421	ILE	2.4
1	E	442	HIS	2.4
1	A	322	LEU	2.4
2	B	115	TRP	2.4
2	F	286	ASN	2.4
1	A	194	GLY	2.4
1	A	334	MET	2.4
1	E	614	GLY	2.4
2	B	159	GLY	2.4
2	F	196	ASP	2.4
1	E	627	PHE	2.4
1	A	433	ILE	2.4
2	F	233	LEU	2.4
1	A	501	MET	2.4
1	E	92	SER	2.4
2	F	272	SER	2.4
1	A	294	PHE	2.4
1	A	536	ASP	2.4
2	F	148	ASP	2.4
2	F	141	LEU	2.4
2	F	239	GLU	2.4
1	E	83	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	174	SER	2.4
2	B	276	LYS	2.4
2	F	113	VAL	2.4
3	G	103	THR	2.4
4	H	57	LEU	2.4
1	A	572	TYR	2.4
1	A	398	ALA	2.4
1	E	112	MET	2.4
1	A	454	TRP	2.4
1	A	476	PRO	2.4
3	C	62	PHE	2.4
4	D	66	THR	2.4
1	E	368	LYS	2.4
1	A	456	PHE	2.3
1	E	57	GLY	2.3
1	E	182	GLY	2.3
1	E	328	THR	2.3
1	A	70	ARG	2.3
2	F	131	TYR	2.3
2	F	187	ALA	2.3
4	D	80	PHE	2.3
1	A	474	GLY	2.3
4	H	60	LEU	2.3
3	C	182	TRP	2.3
3	G	81	CYS	2.3
4	H	50	PHE	2.3
1	E	390	GLY	2.3
2	B	49	ARG	2.3
2	F	49	ARG	2.3
1	E	550	ALA	2.3
2	B	93	LEU	2.3
3	C	153	PHE	2.3
1	A	606	GLU	2.3
1	E	446	GLU	2.3
1	E	586	SER	2.3
2	B	246	HIS	2.3
3	C	120	HIS	2.3
1	A	273	ASN	2.3
3	C	52	THR	2.3
4	H	70	ASN	2.3
3	G	189	TRP	2.3
1	A	116	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	287	ILE	2.3
1	A	430	ALA	2.3
1	E	156	PHE	2.3
3	C	184	PHE	2.3
2	B	211	SER	2.3
2	B	215	LYS	2.3
1	E	243	THR	2.3
2	B	77	LEU	2.3
1	A	373	PHE	2.3
1	A	580	ILE	2.3
1	A	126	GLN	2.3
1	E	505	GLY	2.3
3	C	112	GLY	2.3
2	F	251	ASP	2.3
3	G	143	THR	2.2
2	F	288	PHE	2.2
1	E	633	TYR	2.2
2	F	146	SER	2.2
2	B	261	GLU	2.2
1	E	223	MET	2.2
1	E	476	PRO	2.2
1	E	531	VAL	2.2
2	B	33	GLY	2.2
2	F	250	VAL	2.2
1	A	139	ASN	2.2
1	A	417	HIS	2.2
1	E	294	PHE	2.2
2	B	27	PHE	2.2
1	A	278	TRP	2.2
1	E	443	LYS	2.2
1	A	475	MET	2.2
1	A	159	GLY	2.2
1	E	196	GLY	2.2
1	A	298	ILE	2.2
1	E	421	ILE	2.2
2	B	25	ILE	2.2
2	F	25	ILE	2.2
1	A	276	TRP	2.2
2	B	197	GLN	2.2
1	A	178	SER	2.2
1	E	250	SER	2.2
2	F	258	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
3	G	197	TYR	2.2
4	D	65	MET	2.2
1	E	101	THR	2.2
3	C	81	CYS	2.2
4	D	62	PHE	2.2
1	A	42	TRP	2.2
4	D	61	MET	2.2
1	E	118	LEU	2.2
1	E	547	TYR	2.2
1	A	266	GLY	2.2
1	E	503	GLY	2.2
2	B	160	GLY	2.2
1	A	87	ASN	2.2
1	A	382	ALA	2.2
1	E	176	ASP	2.2
1	A	439	MET	2.2
1	E	342	SER	2.2
2	F	16	GLN	2.2
2	F	143	LYS	2.2
3	G	71	THR	2.2
1	A	412	LEU	2.2
1	E	401	ALA	2.1
3	G	106	LEU	2.2
2	B	19	ASP	2.1
1	E	135	PRO	2.1
1	E	281	PRO	2.1
1	E	460	PHE	2.1
2	B	65	THR	2.1
2	F	259	ALA	2.1
3	G	123	HIS	2.1
1	A	483	GLY	2.1
1	E	75	GLY	2.1
2	F	128	THR	2.1
2	F	224	THR	2.1
1	E	229	LEU	2.1
2	F	20	LEU	2.1
1	A	174	SER	2.1
4	D	89	VAL	2.1
1	A	366	MET	2.1
3	C	80	THR	2.1
4	H	72	THR	2.1
1	A	169	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
3	G	59	ASP	2.1
2	F	263	ARG	2.1
1	A	384	ILE	2.1
1	E	80	ALA	2.1
1	A	383	PHE	2.1
2	F	186	ASN	2.1
1	E	581	HIS	2.1
1	A	347	THR	2.1
1	E	413	VAL	2.1
3	G	58	PRO	2.0
1	A	333	THR	2.0
1	E	409	THR	2.0
1	E	567	GLU	2.0
3	G	146	THR	2.0
1	E	311	ALA	2.0
3	C	84	ALA	2.0
2	F	157	GLN	2.0
4	H	65	MET	2.0
1	E	431	GLY	2.0
2	F	97	PRO	2.0
1	A	494	ILE	2.0
1	A	46	GLU	2.0
1	A	143	TRP	2.0
1	A	277	ILE	2.0
2	B	192	GLU	2.0
1	A	320	SER	2.0
1	E	453	PHE	2.0
2	B	149	SER	2.0
4	D	90	LEU	2.0
2	B	157	GLN	2.0
1	A	386	ASN	2.0
4	D	88	ILE	2.0
1	E	35	THR	2.0
3	G	168	THR	2.0
1	A	566	GLU	2.0
3	G	134	TRP	2.0
1	E	91	ASP	2.0
2	B	213	VAL	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

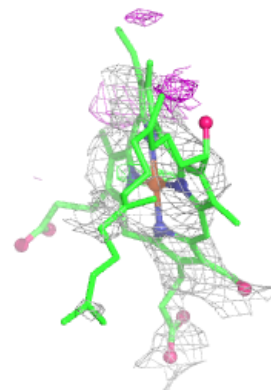
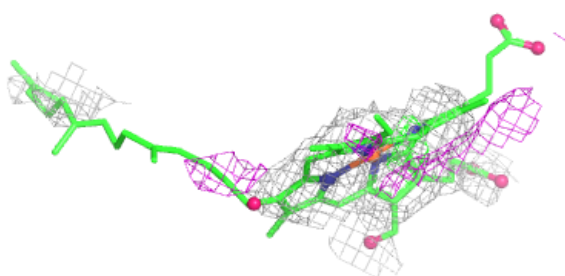
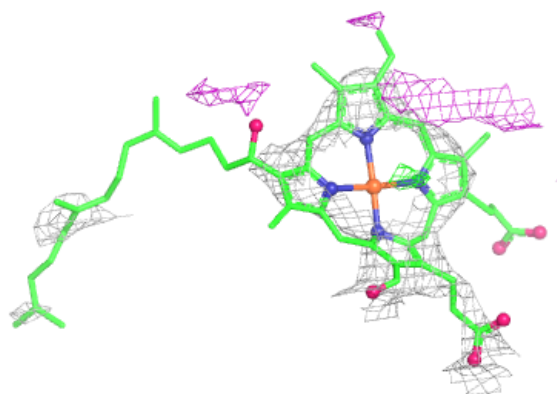
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	HEA	A	1001	60/60	0.91	0.26	80,129,190,212	0
5	HEA	E	1001	60/60	0.91	0.24	81,131,169,173	0
6	CU	A	1003	1/1	0.91	0.13	146,146,146,146	0
5	HEA	E	1002	60/60	0.92	0.24	76,131,152,168	0
5	HEA	A	1002	60/60	0.92	0.29	100,143,198,223	0
7	IHQ	E	1004	14/20	0.94	0.14	106,113,138,146	0
6	CU	E	1003	1/1	0.95	0.08	114,114,114,114	0
7	IHQ	A	1004	14/20	0.97	0.11	76,109,123,159	0

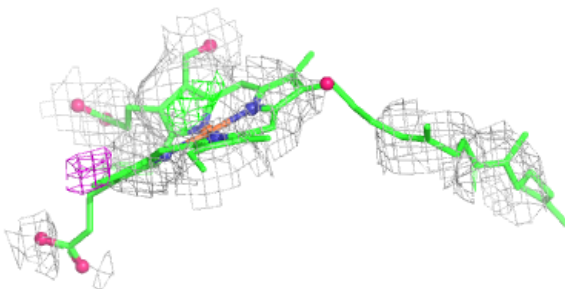
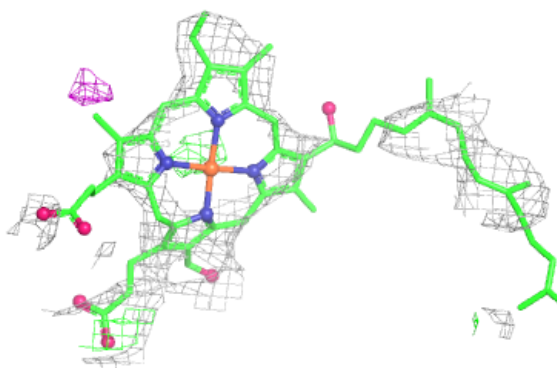
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEA A 1001:

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

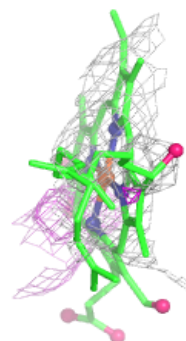
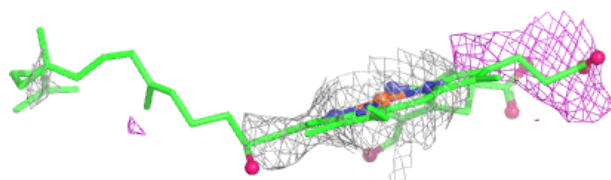
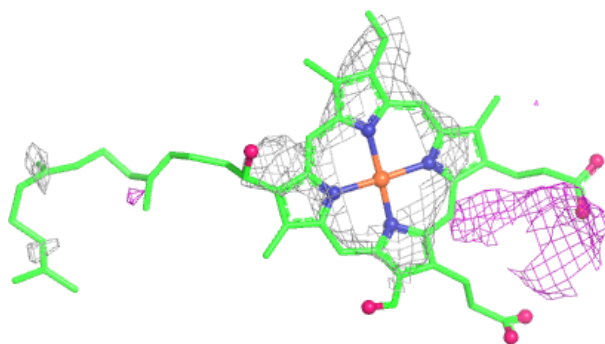
**Electron density around HEA E 1001:**

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

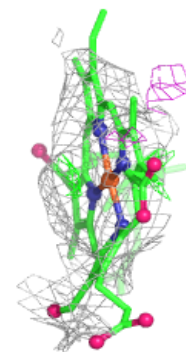
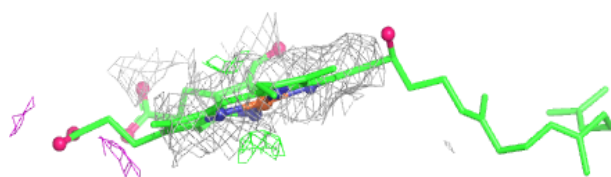
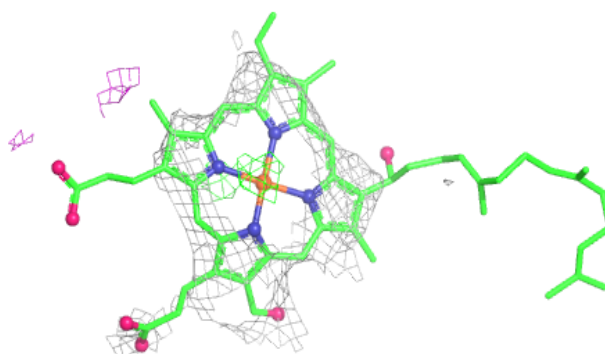


Electron density around HEA E 1002:

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

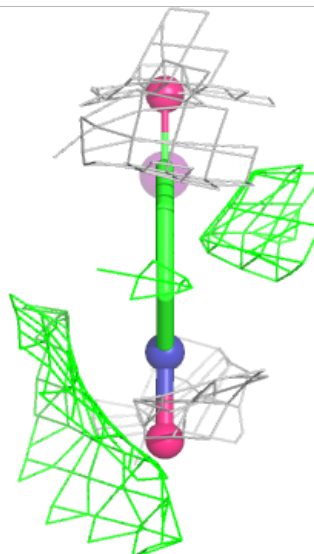
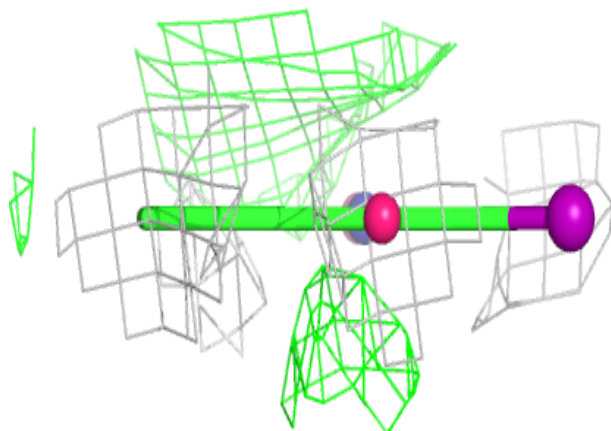
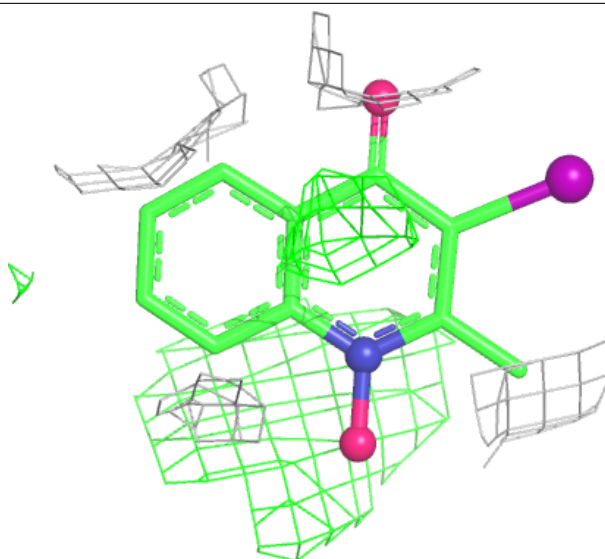
**Electron density around HEA A 1002:**

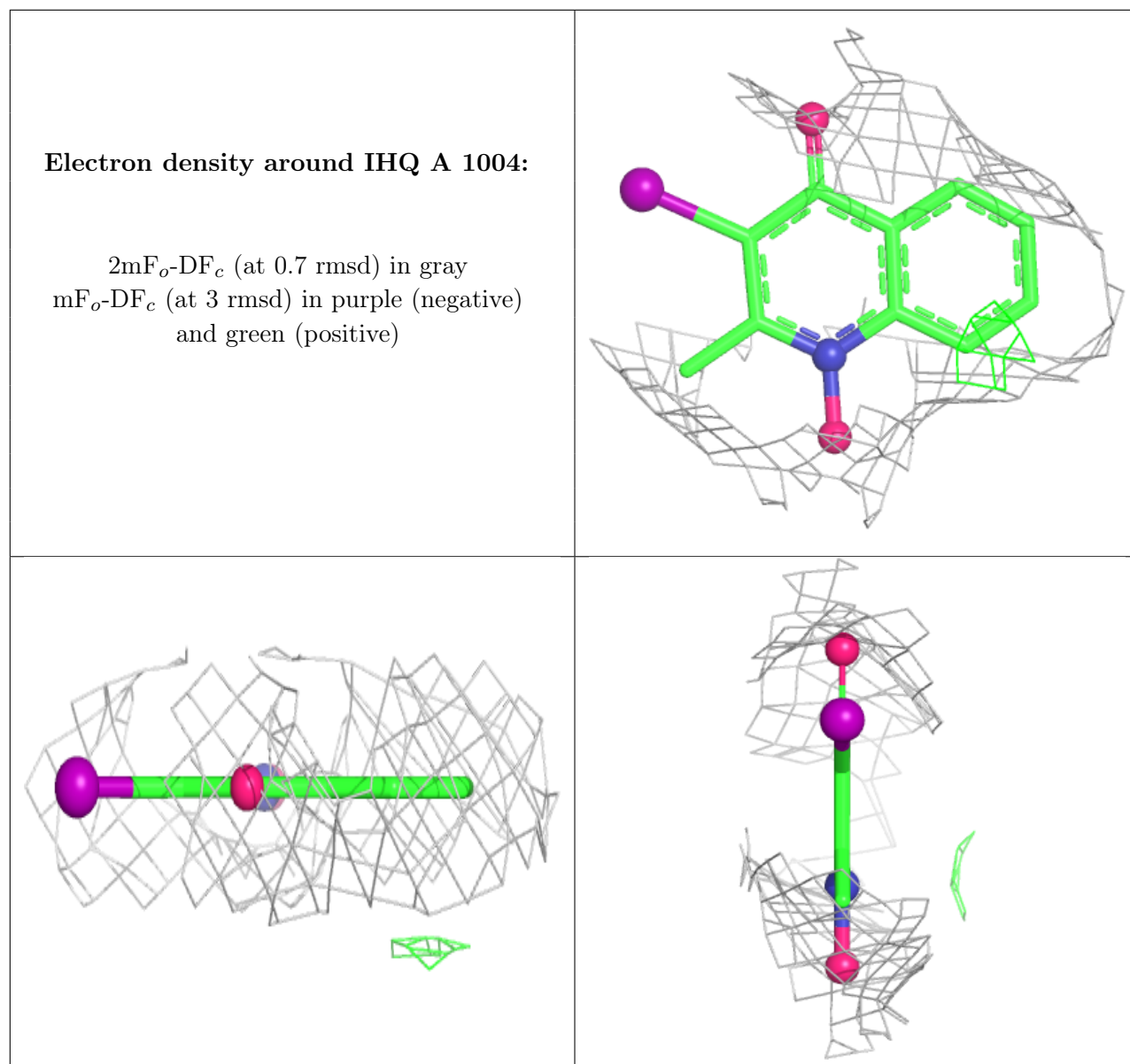
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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.