



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:16 am BST

PDB ID : 6KOE
Title : X-ray Structure of the proton-pumping cytochrome aa3-600 menaquinol oxidase from *Bacillus subtilis*
Authors : Xu, J.; Ding, Z.; Liu, B.; Li, J.; Gennis, R.B.; Zhu, J.
Deposited on : 2019-08-09
Resolution : 3.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

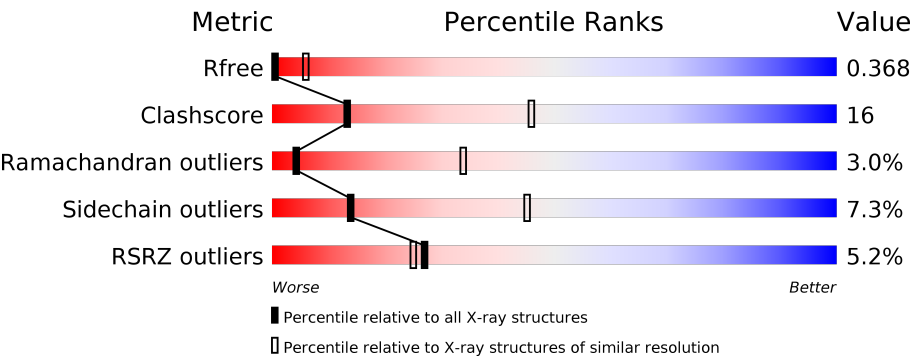
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1039 (3.94-3.58)
Clashscore	141614	1051 (3.92-3.60)
Ramachandran outliers	138981	1015 (3.92-3.60)
Sidechain outliers	138945	1011 (3.92-3.60)
RSRZ outliers	127900	1050 (3.96-3.56)

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

Mol	Chain	Length	Quality of chain
1	A	655	<div><div>2%</div><div><div></div><div>56%</div><div>32%</div><div>•</div><div>7%</div></div></div>
1	E	655	<div><div>3%</div><div><div></div><div>57%</div><div>32%</div><div>•</div><div>7%</div></div></div>
2	B	296	<div><div>10%</div><div><div></div><div>47%</div><div>33%</div><div>6%</div><div>14%</div></div></div>
2	F	296	<div><div>7%</div><div><div></div><div>51%</div><div>29%</div><div>7%</div><div>14%</div></div></div>
3	C	204	<div><div>4%</div><div><div></div><div>61%</div><div>24%</div><div>•</div><div>13%</div></div></div>
3	G	204	<div><div>6%</div><div><div></div><div>64%</div><div>20%</div><div>•</div><div>13%</div></div></div>

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Mol	Chain	Length	Quality of chain
4	D	124	
4	H	124	

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	1001	X	-	-	-
5	HEA	A	1002	X	-	-	X
5	HEA	E	1001	X	-	-	X
5	HEA	E	1002	X	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17910 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			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	650	HIS	-	expression tag	UNP A0A063X8D0
A	651	HIS	-	expression tag	UNP A0A063X8D0
A	652	HIS	-	expression tag	UNP A0A063X8D0
A	653	HIS	-	expression tag	UNP A0A063X8D0
A	654	HIS	-	expression tag	UNP A0A063X8D0
A	655	HIS	-	expression tag	UNP A0A063X8D0
E	650	HIS	-	expression tag	UNP A0A063X8D0
E	651	HIS	-	expression tag	UNP A0A063X8D0
E	652	HIS	-	expression tag	UNP A0A063X8D0
E	653	HIS	-	expression tag	UNP A0A063X8D0
E	654	HIS	-	expression tag	UNP A0A063X8D0
E	655	HIS	-	expression tag	UNP A0A063X8D0

- 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			

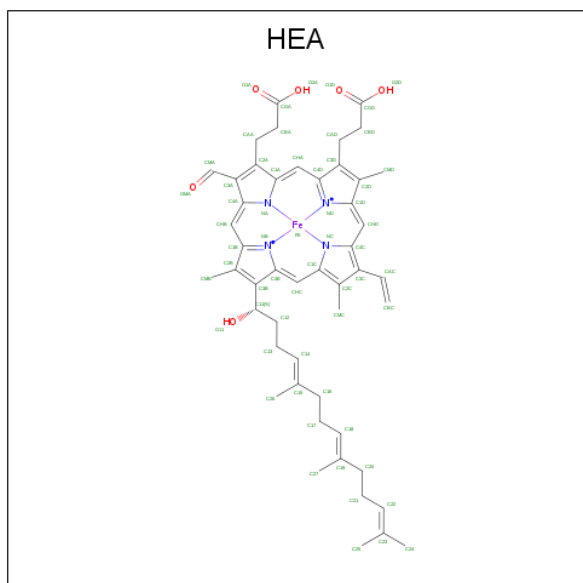
- Molecule 3 is a protein called AA3-600 quinol oxidase subunit IIII.

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 AA3-600 quinol oxidase subunit IV.

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 (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).

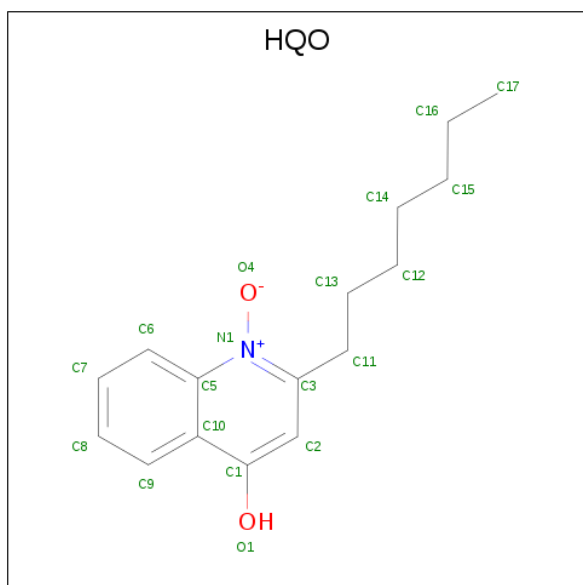


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
5	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
5	E	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
5	E	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

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

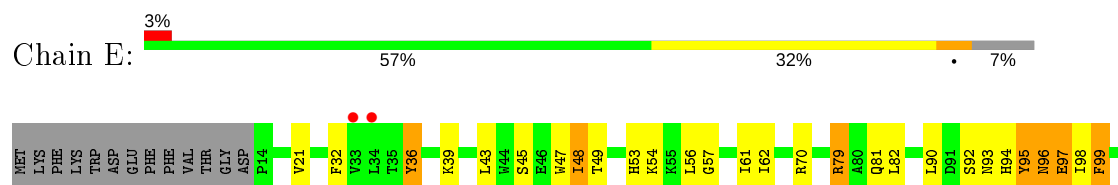
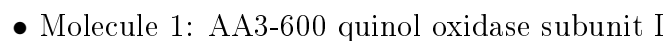
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cu 1 1	0	0
6	E	1	Total Cu 1 1	0	0

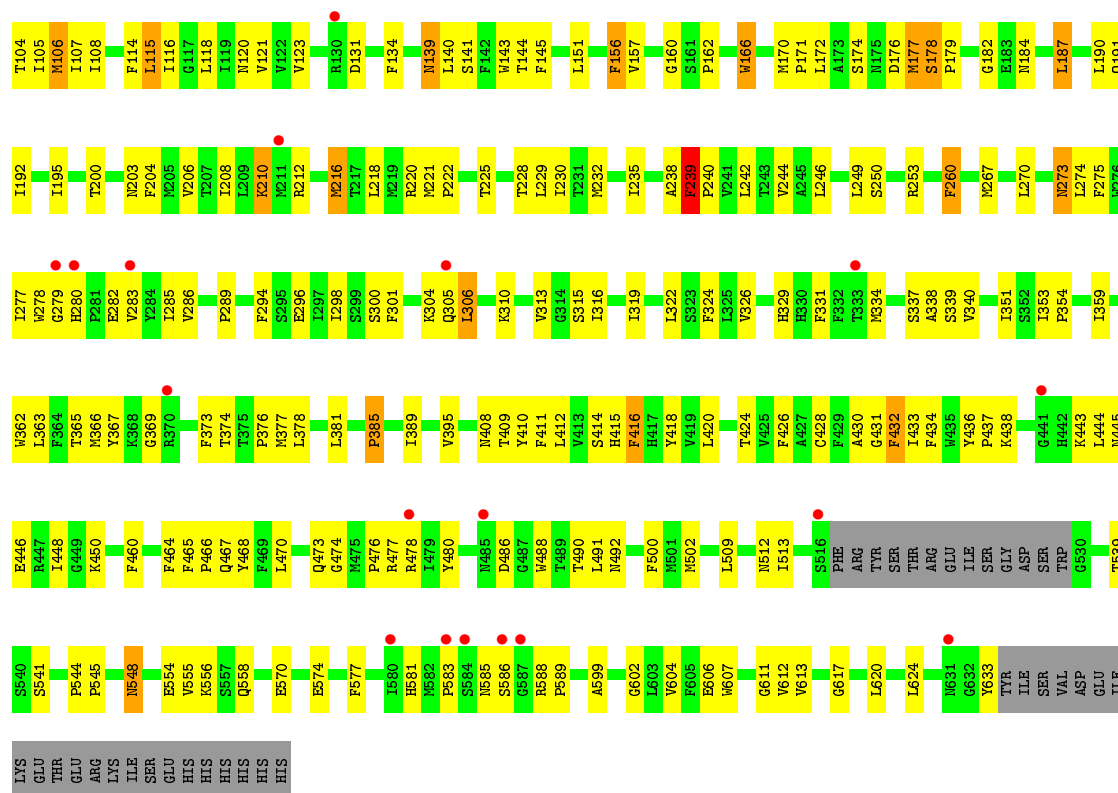
- Molecule 7 is 2-HEPTYL-4-HYDROXY QUINOLINE N-OXIDE (three-letter code: HQO) (formula: C₁₆H₂₁NO₂).



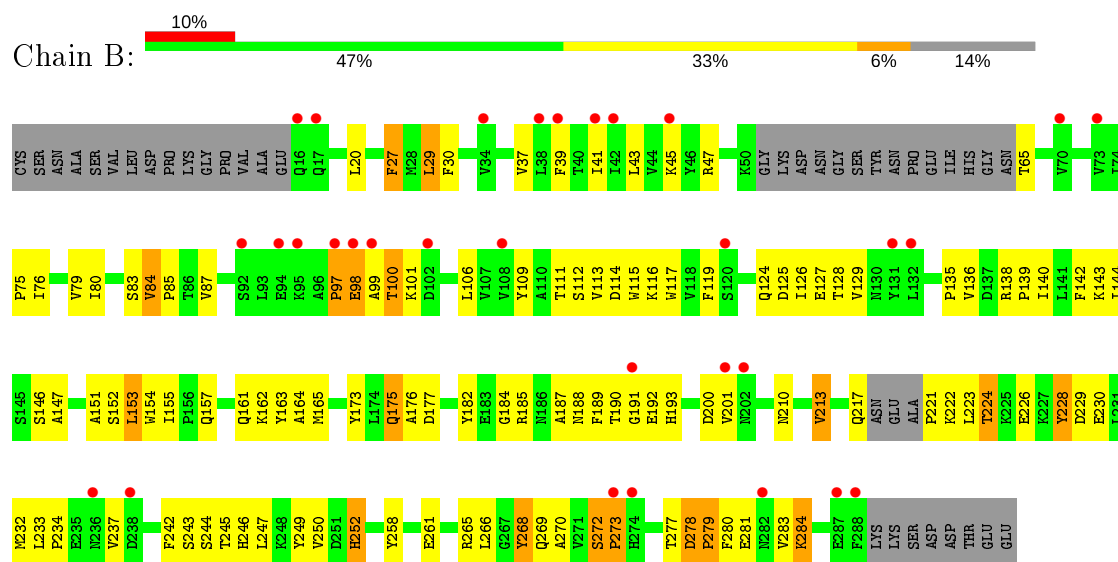
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 13 10 1 2	0	0
7	E	1	Total C N O 13 10 1 2	0	0

- Molecule 1: AA3-600 quinol oxidase subunit I

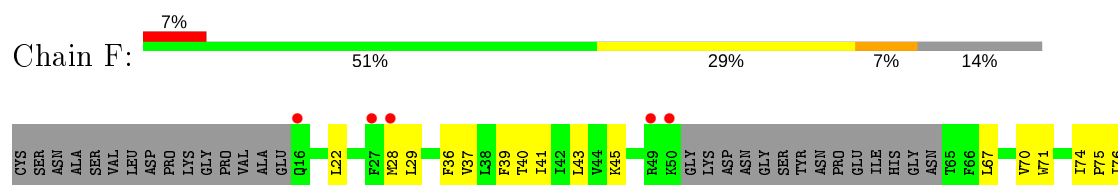


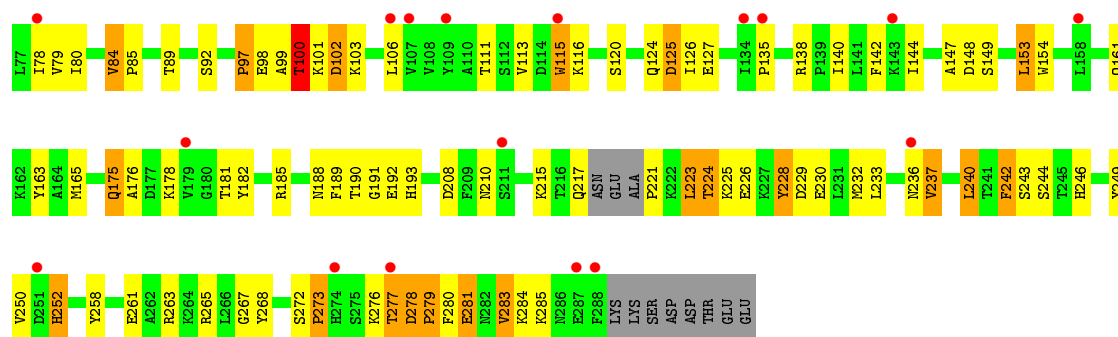


- Molecule 2: Quinol oxidase subunit 2

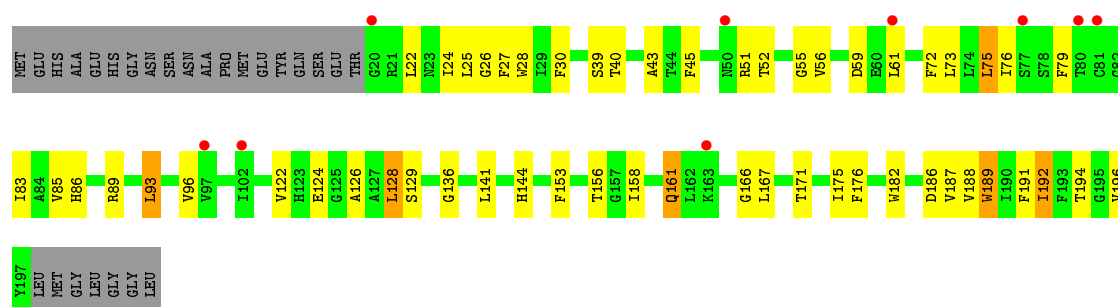


- Molecule 2: Quinol oxidase subunit 2

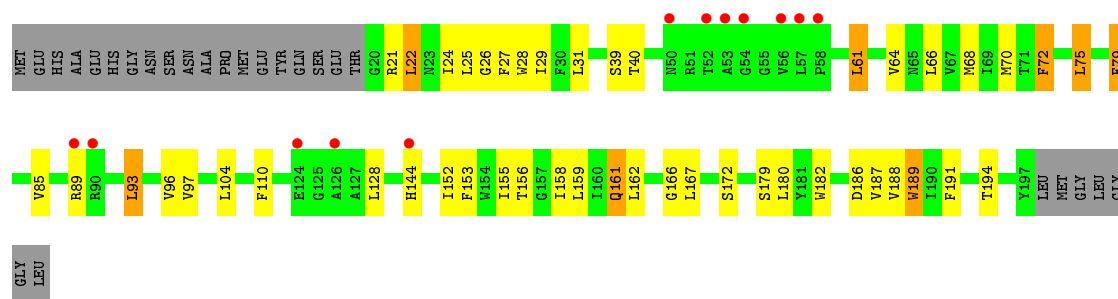




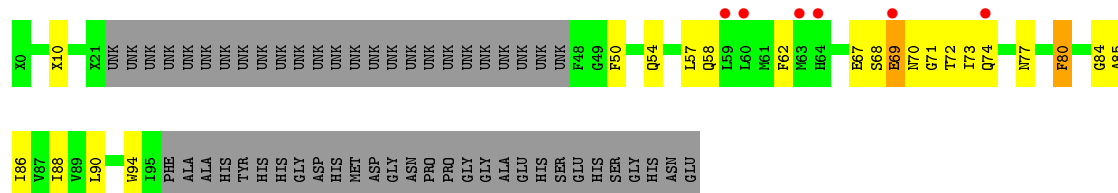
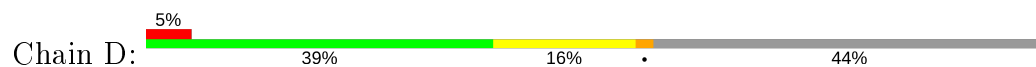
• Molecule 3: AA3-600 quinol oxidase subunit IIII



• Molecule 3: AA3-600 quinol oxidase subunit IIII

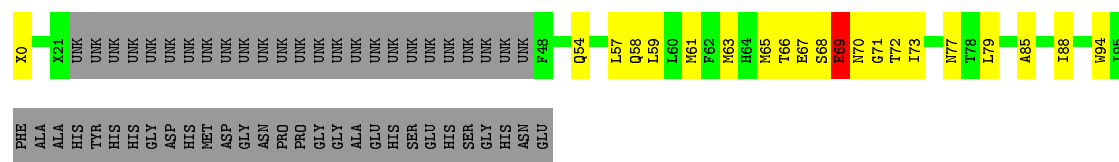
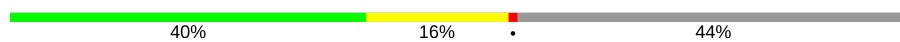


• Molecule 4: AA3-600 quinol oxidase subunit IV



• Molecule 4: AA3-600 quinol oxidase subunit IV

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.99Å 162.11Å 149.51Å 90.00° 109.02° 90.00°	Depositor
Resolution (Å)	49.25 – 3.75 49.25 – 3.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.25-3.75) 99.1 (49.25-3.75)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.14_3235	Depositor
R, R_{free}	0.347 , 0.368 0.347 , 0.368	Depositor DCC
R_{free} test set	1993 reflections (3.85%)	wwPDB-VP
Wilson B-factor (Å ²)	95.0	Xtriage
Anisotropy	0.746	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , -1.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	17910	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: HEA, CU, HQO

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	0.28	0/5022	0.45	0/6827
1	E	0.29	0/5022	0.45	0/6827
2	B	0.27	0/2122	0.48	0/2879
2	F	0.28	0/2122	0.50	0/2879
3	C	0.27	0/1452	0.44	0/1974
3	G	0.26	0/1452	0.44	0/1974
4	D	0.30	0/381	0.45	0/514
4	H	0.29	0/381	0.44	0/514
All	All	0.28	0/17954	0.46	0/24388

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	184	0
1	E	4855	0	4855	173	0
2	B	2073	0	2061	82	0
2	F	2073	0	2061	73	0
3	C	1411	0	1444	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1411	0	1444	43	0
4	D	482	0	395	16	0
4	H	482	0	395	22	0
5	A	120	0	106	18	0
5	E	120	0	106	12	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
7	A	13	0	4	4	0
7	E	13	0	5	5	0
All	All	17910	0	17731	577	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 16.

All (577) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:MET:HG2	1:A:260:PHE:HB2	1.51	0.92
1:E:170:MET:HG2	1:E:260:PHE:HB2	1.56	0.88
1:E:108:ILE:HG21	1:E:190:LEU:HD22	1.61	0.83
1:A:187:LEU:HD21	1:A:249:LEU:HG	1.63	0.81
1:A:134:PHE:HZ	3:C:26:GLY:HA3	1.42	0.81
2:B:261:GLU:O	2:B:265:ARG:NH2	2.13	0.80
1:E:39:LYS:HE3	1:E:43:LEU:HB2	1.67	0.77
1:A:39:LYS:HE3	1:A:43:LEU:HB2	1.65	0.77
1:A:79:ARG:HH22	1:A:495:SER:HB3	1.50	0.77
1:E:409:THR:HA	1:E:476:PRO:HA	1.68	0.76
1:E:326:VAL:O	1:E:329:HIS:ND1	2.18	0.75
2:F:284:LYS:HD3	2:F:285:LYS:H	1.52	0.75
2:F:116:LYS:HD3	2:F:237:VAL:HG11	1.67	0.74
1:E:273:ASN:HA	1:E:331:PHE:HZ	1.52	0.74
1:E:409:THR:O	1:E:411:PHE:N	2.20	0.74
1:A:108:ILE:HG21	1:A:190:LEU:HD22	1.70	0.74
1:E:54:LYS:NZ	1:E:545:PRO:O	2.20	0.74
2:F:229:ASP:OD2	2:F:265:ARG:NH1	2.20	0.74
1:E:94:HIS:HD2	7:E:1004:HQO:HC9	1.51	0.73
1:A:409:THR:O	1:A:411:PHE:N	2.21	0.73
2:B:229:ASP:OD2	2:B:265:ARG:NH1	2.21	0.73
1:E:82:LEU:O	1:E:492:ASN:ND2	2.22	0.73
1:A:54:LYS:NZ	1:A:545:PRO:O	2.21	0.71
2:F:102:ASP:N	2:F:102:ASP:OD2	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:VAL:HG21	1:A:228:THR:HG21	1.71	0.71
1:A:467:GLN:HA	1:A:470:LEU:HB2	1.71	0.70
2:B:76:ILE:HA	2:B:79:VAL:HG22	1.73	0.70
4:D:50:PHE:O	4:D:54:GLN:NE2	2.24	0.70
3:C:122:VAL:HA	3:C:126:ALA:HB2	1.72	0.70
3:C:85:VAL:HA	3:C:89:ARG:HB2	1.74	0.70
1:A:53:HIS:HD2	1:A:131:ASP:HA	1.55	0.70
1:A:326:VAL:HG22	1:A:329:HIS:HD2	1.57	0.69
1:E:187:LEU:HD21	1:E:249:LEU:HG	1.72	0.69
1:E:230:ILE:HG13	1:E:316:ILE:HG23	1.72	0.69
2:B:221:PRO:O	2:B:243:SER:OG	2.09	0.69
1:E:97:GLU:HB2	7:E:1004:HQO:HC8	1.76	0.68
2:B:175:GLN:NE2	2:B:176:ALA:O	2.26	0.68
2:B:230:GLU:O	2:B:284:LYS:NZ	2.23	0.68
1:A:246:LEU:O	1:A:250:SER:N	2.20	0.68
1:E:56:LEU:HD21	1:E:139:ASN:HA	1.74	0.68
1:A:134:PHE:CZ	3:C:26:GLY:HA3	2.27	0.68
1:E:467:GLN:HA	1:E:470:LEU:HB2	1.75	0.68
1:A:286:VAL:O	1:A:424:THR:OG1	2.11	0.68
1:E:470:LEU:HD11	1:E:492:ASN:HA	1.74	0.68
2:F:37:VAL:HG13	2:F:41:ILE:HD12	1.76	0.68
1:E:408:ASN:HB3	1:E:477:ARG:HG2	1.76	0.68
1:A:584:SER:HG	1:A:633:TYR:HH	1.42	0.67
1:A:322:LEU:HB3	1:A:351:ILE:HD12	1.75	0.67
2:F:75:PRO:HB2	1:E:353:ILE:HD12	1.76	0.67
1:E:378:LEU:HD23	1:E:381:LEU:HD12	1.78	0.66
1:A:376:PRO:HG3	1:A:433:ILE:HG22	1.78	0.66
2:F:261:GLU:O	2:F:265:ARG:NH2	2.29	0.66
1:A:337:SER:O	1:A:339:SER:N	2.29	0.66
3:C:186:ASP:HA	3:C:189:TRP:HB2	1.77	0.66
1:A:94:HIS:NE2	7:A:1004:HQO:O1	2.28	0.66
1:A:20:GLN:O	1:A:24:ALA:N	2.25	0.66
3:C:75:LEU:HD11	3:C:182:TRP:HE1	1.60	0.65
1:E:106:MET:O	1:E:108:ILE:N	2.28	0.65
1:A:599:ALA:HB2	1:A:617:GLY:HA3	1.77	0.65
1:E:242:LEU:HB2	1:E:278:TRP:CG	2.32	0.65
1:A:106:MET:O	1:A:108:ILE:N	2.30	0.65
2:F:175:GLN:NE2	2:F:176:ALA:O	2.30	0.65
1:E:286:VAL:O	1:E:424:THR:OG1	2.14	0.64
2:F:178:LYS:O	2:F:182:TYR:OH	2.13	0.64
1:A:53:HIS:CD2	1:A:131:ASP:HA	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:GLU:HB2	7:A:1004:HQO:HC8	1.79	0.64
3:C:22:LEU:H	3:C:22:LEU:HD23	1.61	0.64
1:E:539:THR:HG21	1:E:544:PRO:HG3	1.80	0.64
1:E:53:HIS:HD2	1:E:131:ASP:HA	1.63	0.64
1:A:173:ALA:O	1:A:253:ARG:NH1	2.31	0.64
1:A:334:MET:HA	2:B:163:TYR:HB2	1.79	0.64
2:F:148:ASP:OD2	2:F:263:ARG:NH2	2.30	0.63
1:A:409:THR:HA	1:A:476:PRO:HA	1.79	0.63
1:A:123:VAL:HG13	1:A:225:THR:HG23	1.79	0.63
1:E:57:GLY:HA3	1:E:121:VAL:HG23	1.80	0.62
1:E:220:ARG:HB3	1:E:558:GLN:HG3	1.81	0.62
2:B:114:ASP:HB3	2:B:234:PRO:HB3	1.80	0.62
1:A:378:LEU:HD23	1:A:381:LEU:HD12	1.81	0.62
2:B:233:LEU:HD13	2:B:284:LYS:HZ3	1.64	0.62
2:B:278:ASP:O	2:B:280:PHE:N	2.32	0.62
2:B:155:ILE:HA	2:B:184:GLY:HA2	1.82	0.62
1:E:554:GLU:HB3	1:E:556:LYS:HE3	1.82	0.62
1:E:420:LEU:HD13	5:E:1002:HEA:HBC2	1.82	0.62
1:E:123:VAL:HG13	1:E:225:THR:HG23	1.82	0.62
4:D:71:GLY:O	4:D:73:ILE:N	2.33	0.61
1:E:322:LEU:HB3	1:E:351:ILE:HD12	1.82	0.61
2:B:142:PHE:HB3	2:B:144:ILE:HD11	1.83	0.61
3:C:43:ALA:HB2	4:D:88:ILE:HG22	1.81	0.61
2:F:224:THR:O	2:F:226:GLU:N	2.31	0.60
2:F:267:GLY:HA3	2:F:281:GLU:HG3	1.83	0.60
3:G:79:PHE:HE2	3:G:179:SER:HA	1.66	0.60
2:B:151:ALA:O	2:B:164:ALA:N	2.23	0.60
1:E:326:VAL:HG22	1:E:329:HIS:HD1	1.66	0.60
1:A:353:ILE:HD12	2:B:75:PRO:HB2	1.82	0.60
2:B:224:THR:O	2:B:226:GLU:N	2.35	0.60
1:E:359:ILE:HA	1:E:362:TRP:CE3	2.37	0.60
1:A:177:MET:HG2	1:A:179:PRO:HD2	1.83	0.60
1:E:373:PHE:CD1	1:E:381:LEU:HD11	2.36	0.60
1:E:445:ASN:HB3	1:E:448:ILE:HD11	1.82	0.59
2:F:228:TYR:HD2	2:F:249:TYR:HD2	1.48	0.59
1:A:110:MET:O	1:A:114:PHE:HB2	2.02	0.59
3:C:188:VAL:O	3:C:192:ILE:N	2.35	0.59
1:E:315:SER:OG	1:E:354:PRO:O	2.19	0.59
3:G:96:VAL:HB	3:G:162:LEU:HD11	1.84	0.59
1:E:53:HIS:CD2	1:E:131:ASP:HA	2.37	0.59
1:A:212:ARG:HH12	1:A:218:LEU:HD12	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:SER:O	1:A:96:ASN:ND2	2.36	0.58
1:E:96:ASN:HD22	1:E:96:ASN:N	2.01	0.58
3:G:186:ASP:HA	3:G:189:TRP:HB2	1.83	0.58
2:B:112:SER:H	2:B:146:SER:HA	1.68	0.58
1:E:377:MET:O	1:E:381:LEU:N	2.29	0.58
1:E:426:PHE:O	1:E:430:ALA:N	2.30	0.58
1:E:54:LYS:NZ	1:E:544:PRO:HB2	2.19	0.58
1:E:416:PHE:CZ	5:E:1001:HEA:HHD	2.38	0.58
2:B:99:ALA:HB1	2:B:139:PRO:HG3	1.86	0.58
2:F:221:PRO:O	2:F:243:SER:OG	2.12	0.58
1:E:414:SER:OG	1:E:464:PHE:O	2.18	0.58
3:G:156:THR:HA	3:G:159:LEU:HB2	1.86	0.58
1:E:242:LEU:HB2	1:E:278:TRP:CD1	2.38	0.58
1:A:346:ILE:HD11	2:B:87:VAL:HG21	1.86	0.58
1:A:476:PRO:HG3	2:B:154:TRP:HZ3	1.68	0.58
1:A:554:GLU:HB3	1:A:556:LYS:HE3	1.86	0.57
1:E:140:LEU:HB3	1:E:589:PRO:HB3	1.85	0.57
1:A:49:THR:OG1	1:A:586:SER:O	2.20	0.57
2:F:154:TRP:HZ3	1:E:476:PRO:HG3	1.69	0.57
2:F:190:THR:HG21	1:E:99:PHE:CE1	2.39	0.57
1:A:184:ASN:HB3	1:A:604:VAL:HG22	1.87	0.57
2:B:97:PRO:O	2:B:99:ALA:N	2.37	0.57
1:E:94:HIS:CD2	7:E:1004:HQO:HC9	2.37	0.57
1:E:599:ALA:HB2	1:E:617:GLY:HA3	1.86	0.57
2:F:230:GLU:O	2:F:284:LYS:NZ	2.38	0.57
2:B:109:TYR:HA	2:B:143:LYS:HB2	1.86	0.57
1:E:337:SER:O	1:E:339:SER:N	2.36	0.57
2:F:268:TYR:CD1	2:F:279:PRO:HD2	2.39	0.57
2:F:268:TYR:HD1	2:F:279:PRO:HD2	1.69	0.57
3:C:141:LEU:HA	3:C:144:HIS:HB3	1.85	0.57
2:F:272:SER:OG	2:F:273:PRO:HD3	2.04	0.57
2:B:269:GLN:NE2	2:F:281:GLU:OE2	2.37	0.57
1:E:174:SER:HA	1:E:253:ARG:HH11	1.69	0.56
2:F:190:THR:HB	1:E:478:ARG:HB3	1.86	0.56
4:H:71:GLY:O	4:H:73:ILE:N	2.38	0.56
1:A:420:LEU:O	1:A:424:THR:N	2.35	0.56
1:E:49:THR:OG1	1:E:586:SER:O	2.23	0.56
1:E:602:GLY:HA3	1:E:613:VAL:HG23	1.87	0.56
1:E:607:TRP:HE1	1:E:612:VAL:HB	1.70	0.56
1:A:301:PHE:HE1	1:A:531:VAL:H	1.54	0.56
1:E:607:TRP:HD1	1:E:611:GLY:HA2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LYS:HZ3	1:A:544:PRO:HB2	1.71	0.56
3:C:93:LEU:H	3:C:93:LEU:HD23	1.71	0.56
1:A:470:LEU:HD11	1:A:492:ASN:HA	1.88	0.56
1:E:47:TRP:O	1:E:49:THR:N	2.39	0.56
1:A:344:PHE:O	1:A:348:THR:OG1	2.21	0.55
1:E:115:LEU:HG	1:E:289:PRO:HB2	1.88	0.55
3:G:93:LEU:H	3:G:93:LEU:HD23	1.71	0.55
3:C:153:PHE:HA	3:C:156:THR:HG22	1.88	0.55
3:C:73:LEU:HD12	3:C:76:ILE:HD11	1.87	0.55
2:F:97:PRO:O	2:F:99:ALA:N	2.38	0.55
1:A:284:TYR:HA	1:A:287:ILE:HG22	1.88	0.55
1:A:107:ILE:HA	1:A:111:ALA:HB3	1.88	0.55
1:A:79:ARG:NH2	1:A:467:GLN:OE1	2.35	0.55
4:D:90:LEU:O	4:D:94:TRP:HB2	2.06	0.55
1:A:67:MET:HB3	1:A:105:ILE:HG23	1.88	0.55
2:B:84:VAL:H	2:B:85:PRO:HD2	1.71	0.55
2:F:84:VAL:H	2:F:85:PRO:HD2	1.70	0.55
1:A:136:TYR:OH	1:A:588:ARG:NH1	2.38	0.55
2:F:163:TYR:CZ	2:F:189:PHE:HZ	2.24	0.55
1:A:242:LEU:HB2	1:A:278:TRP:CD1	2.41	0.55
3:G:40:THR:HG23	1:E:274:LEU:HD22	1.88	0.55
2:F:76:ILE:HA	2:F:79:VAL:HG22	1.88	0.55
1:A:119:ILE:HG21	1:A:232:MET:HE2	1.89	0.55
2:B:223:LEU:N	2:B:244:SER:HB3	2.21	0.55
1:A:274:LEU:HD22	3:C:40:THR:HG23	1.89	0.55
1:E:54:LYS:NZ	1:E:548:ASN:HB3	2.22	0.55
1:E:588:ARG:HE	1:E:624:LEU:HB3	1.70	0.55
4:H:70:ASN:OD1	1:E:210:LYS:NZ	2.40	0.54
1:A:120:ASN:HA	1:A:204:PHE:CZ	2.42	0.54
1:E:94:HIS:NE2	7:E:1004:HQO:O1	2.39	0.54
1:E:296:GLU:O	1:E:300:SER:N	2.40	0.54
2:B:111:THR:HG21	2:B:252:HIS:CD2	2.42	0.54
1:E:48:ILE:HA	1:E:143:TRP:HZ2	1.72	0.54
3:G:194:THR:HG21	4:H:54:GLN:HG3	1.89	0.54
1:A:412:LEU:HD11	5:A:1002:HEA:HHA	1.88	0.54
2:B:233:LEU:HD11	2:B:266:LEU:HD12	1.89	0.54
2:B:268:TYR:HD1	2:B:279:PRO:HD2	1.72	0.54
2:F:154:TRP:CZ3	1:E:476:PRO:HG3	2.43	0.54
1:A:204:PHE:HB2	1:A:232:MET:HG3	1.90	0.54
1:A:96:ASN:HA	1:A:99:PHE:CD1	2.42	0.54
1:E:21:VAL:HB	1:E:157:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:MET:HB2	1:E:270:LEU:HB2	1.90	0.54
2:F:43:LEU:HB2	1:E:367:TYR:CZ	2.43	0.54
1:E:437:PRO:HG3	1:E:443:LYS:HB3	1.89	0.54
2:F:185:ARG:HD3	1:E:476:PRO:HG2	1.88	0.54
1:A:476:PRO:HG3	2:B:154:TRP:CZ3	2.43	0.54
2:F:278:ASP:O	2:F:280:PHE:N	2.41	0.54
2:F:190:THR:OG1	1:E:96:ASN:OD1	2.15	0.53
3:G:162:LEU:HD23	3:G:166:GLY:HA2	1.90	0.53
2:F:272:SER:HB3	1:E:179:PRO:HB3	1.91	0.53
3:G:85:VAL:HG21	4:H:0:UNK:N	2.23	0.53
1:A:240:PRO:O	1:A:244:VAL:HG22	2.09	0.53
2:B:106:LEU:HD22	2:B:138:ARG:HH21	1.72	0.53
1:E:428:CYS:O	1:E:432:PHE:HB2	2.08	0.53
1:A:72:GLY:HA2	5:A:1001:HEA:H14	1.90	0.53
1:E:81:GLN:NE2	1:E:480:TYR:O	2.37	0.53
1:A:376:PRO:HB3	1:A:434:PHE:HB2	1.90	0.52
1:A:47:TRP:O	1:A:49:THR:N	2.42	0.52
1:A:54:LYS:NZ	1:A:544:PRO:HB2	2.24	0.52
1:A:259:PHE:HE1	3:C:136:GLY:HA2	1.73	0.52
1:A:120:ASN:HA	1:A:204:PHE:HZ	1.75	0.52
1:A:273:ASN:HA	1:A:331:PHE:HZ	1.75	0.52
1:A:57:GLY:HA3	1:A:121:VAL:HG23	1.91	0.52
2:F:124:GLN:O	2:F:126:ILE:N	2.43	0.52
1:A:446:GLU:O	1:A:450:LYS:HD3	2.09	0.52
2:B:136:VAL:HA	2:B:176:ALA:HB3	1.91	0.52
2:B:223:LEU:H	2:B:244:SER:HB3	1.74	0.52
1:E:280:HIS:CG	1:E:329:HIS:HE1	2.28	0.52
1:E:184:ASN:HB3	1:E:604:VAL:HG22	1.90	0.52
1:A:106:MET:HA	1:A:110:MET:HB3	1.92	0.52
1:E:121:VAL:HG13	1:E:438:LYS:HZ2	1.75	0.52
1:E:362:TRP:O	1:E:366:MET:HB2	2.09	0.52
1:A:69:PHE:CE1	5:A:1001:HEA:H202	2.44	0.52
1:E:294:PHE:HZ	1:E:426:PHE:HB3	1.75	0.52
1:E:96:ASN:HD22	1:E:96:ASN:H	1.56	0.52
2:F:276:LYS:HD2	2:F:278:ASP:H	1.74	0.52
3:C:39:SER:HB2	4:D:85:ALA:HA	1.92	0.51
2:B:144:ILE:HD12	2:B:153:LEU:HD21	1.92	0.51
4:D:84:GLY:O	4:D:88:ILE:N	2.32	0.51
1:E:509:LEU:O	1:E:513:ILE:HG13	2.10	0.51
1:A:107:ILE:O	1:A:112:MET:HB2	2.10	0.51
1:A:304:LYS:HG2	1:A:305:GLN:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ASN:OD1	2:B:190:THR:OG1	2.22	0.51
2:B:157:GLN:HG3	2:B:182:TYR:HA	1.91	0.51
1:A:277:ILE:HD13	4:D:88:ILE:HG12	1.93	0.51
1:E:238:ALA:HB2	1:E:324:PHE:CZ	2.45	0.51
1:A:82:LEU:O	1:A:492:ASN:ND2	2.44	0.51
3:C:192:ILE:O	3:C:196:VAL:HG22	2.09	0.51
3:G:153:PHE:HA	3:G:156:THR:HG22	1.93	0.51
1:A:54:LYS:NZ	1:A:548:ASN:HB3	2.26	0.51
3:C:144:HIS:CE1	3:C:189:TRP:CE2	2.98	0.51
1:E:239:PHE:H	1:E:240:PRO:HD2	1.76	0.51
1:E:54:LYS:HZ1	1:E:548:ASN:HB3	1.75	0.51
1:A:187:LEU:HD11	1:A:249:LEU:HD23	1.93	0.51
1:A:301:PHE:HD2	1:A:377:MET:HG2	1.76	0.51
1:E:79:ARG:NH2	1:E:467:GLN:OE1	2.29	0.51
2:B:163:TYR:CZ	2:B:189:PHE:HZ	2.29	0.51
1:E:235:ILE:HG12	1:E:285:ILE:HD13	1.92	0.51
1:A:367:TYR:C	1:A:369:GLY:H	2.13	0.50
1:A:414:SER:OG	1:A:464:PHE:O	2.17	0.50
2:B:43:LEU:O	2:B:45:LYS:N	2.40	0.50
3:C:188:VAL:HA	3:C:191:PHE:HB2	1.93	0.50
3:G:28:TRP:CZ2	4:H:66:THR:HG22	2.47	0.50
1:A:408:ASN:HB3	1:A:477:ARG:HG2	1.92	0.50
1:E:240:PRO:O	1:E:244:VAL:HG22	2.12	0.50
3:G:24:ILE:O	3:G:28:TRP:HB2	2.11	0.50
4:H:57:LEU:HD22	4:H:58:GLN:NE2	2.27	0.50
1:A:506:PHE:CG	5:A:1001:HEA:H162	2.46	0.50
1:E:588:ARG:NE	1:E:624:LEU:HB3	2.26	0.50
2:F:154:TRP:HA	2:F:161:GLN:HB3	1.94	0.50
3:G:167:LEU:HB3	3:G:172:SER:HB2	1.94	0.50
1:A:530:GLY:HA3	1:A:537:TRP:HZ3	1.76	0.50
3:C:161:GLN:O	3:C:166:GLY:N	2.44	0.50
1:E:160:GLY:O	1:E:182:GLY:HA2	2.11	0.50
3:C:75:LEU:HD11	3:C:182:TRP:NE1	2.24	0.50
3:G:85:VAL:HG21	4:H:0:UNK:H	1.77	0.50
1:A:301:PHE:HB2	1:A:377:MET:SD	2.52	0.50
1:A:56:LEU:HD21	1:A:139:ASN:HA	1.94	0.50
2:F:217:GLN:N	2:F:217:GLN:OE1	2.43	0.50
1:A:194:GLY:HA2	1:A:239:PHE:CE1	2.47	0.49
1:E:235:ILE:O	1:E:239:PHE:HB2	2.12	0.49
1:E:156:PHE:HE1	7:E:1004:HQO:C5	2.24	0.49
4:H:94:TRP:NE1	1:E:340:VAL:HG12	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:61:LEU:HD12	3:G:64:VAL:H	1.78	0.49
1:A:539:THR:HG21	1:A:544:PRO:HG3	1.94	0.49
2:B:135:PRO:HG2	2:B:138:ARG:HD2	1.93	0.49
3:C:194:THR:HG21	4:D:54:GLN:HG3	1.93	0.49
1:E:187:LEU:HD23	1:E:250:SER:HA	1.94	0.49
1:A:96:ASN:HD22	1:A:96:ASN:H	1.61	0.49
1:E:141:SER:OG	1:E:200:THR:OG1	2.26	0.49
2:F:89:THR:HA	2:F:92:SER:HB3	1.94	0.49
3:G:28:TRP:HZ2	4:H:66:THR:HG22	1.78	0.49
1:E:420:LEU:HD13	5:E:1002:HEA:CBC	2.43	0.49
2:B:79:VAL:O	2:B:83:SER:N	2.41	0.49
1:A:420:LEU:HD13	5:A:1002:HEA:HBC2	1.94	0.49
2:B:250:VAL:O	2:B:252:HIS:N	2.43	0.49
1:E:607:TRP:HD1	1:E:612:VAL:H	1.56	0.48
3:G:22:LEU:O	3:G:26:GLY:N	2.28	0.48
2:B:250:VAL:C	2:B:252:HIS:H	2.17	0.48
1:E:177:MET:HG2	1:E:179:PRO:HD2	1.94	0.48
2:F:101:LYS:HE3	2:F:102:ASP:OD2	2.13	0.48
1:A:254:LEU:HD21	1:A:603:LEU:HB3	1.94	0.48
1:A:607:TRP:HE1	1:A:612:VAL:HB	1.77	0.48
1:E:606:GLU:HB3	1:E:607:TRP:CE3	2.48	0.48
2:F:223:LEU:HD22	2:F:225:LYS:H	1.78	0.48
1:A:191:GLN:OE1	1:A:246:LEU:HB2	2.14	0.48
1:E:280:HIS:HA	1:E:283:VAL:HB	1.95	0.48
2:F:100:THR:OG1	2:F:101:LYS:N	2.45	0.48
1:A:95:TYR:HA	1:A:98:ILE:HB	1.94	0.48
5:E:1001:HEA:HMC1	5:E:1001:HEA:HBC1	1.94	0.48
1:E:301:PHE:HD2	1:E:377:MET:HG2	1.78	0.48
3:C:51:ARG:O	3:C:52:THR:OG1	2.29	0.48
2:B:223:LEU:HD11	2:B:249:TYR:CE2	2.49	0.48
3:G:26:GLY:HA3	1:E:134:PHE:HZ	1.77	0.48
1:A:72:GLY:HA3	5:A:1001:HEA:H161	1.96	0.48
1:A:476:PRO:HG2	2:B:185:ARG:HD3	1.96	0.48
2:B:140:ILE:O	2:B:173:TYR:HA	2.14	0.48
2:B:245:THR:HG22	2:B:247:LEU:H	1.78	0.48
2:F:223:LEU:N	2:F:244:SER:HB3	2.29	0.48
3:G:39:SER:HB2	4:H:85:ALA:HA	1.95	0.48
1:E:460:PHE:HA	1:E:502:MET:SD	2.53	0.47
2:F:135:PRO:HG2	2:F:138:ARG:HD2	1.96	0.47
3:G:75:LEU:HD11	3:G:182:TRP:NE1	2.29	0.47
1:A:116:ILE:O	1:A:120:ASN:N	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:LEU:O	1:A:513:ILE:HG13	2.15	0.47
1:E:212:ARG:HH12	1:E:218:LEU:HD12	1.79	0.47
2:F:67:LEU:O	2:F:70:VAL:HG12	2.13	0.47
3:G:161:GLN:OE1	3:G:162:LEU:HG	2.13	0.47
2:B:98:GLU:O	2:B:175:GLN:HB2	2.14	0.47
4:H:68:SER:O	4:H:70:ASN:N	2.47	0.47
1:A:368:LYS:H	2:B:47:ARG:NH1	2.12	0.47
1:A:432:PHE:HB3	1:A:433:ILE:HD12	1.97	0.47
1:A:96:ASN:HD22	1:A:96:ASN:N	2.13	0.47
2:B:217:GLN:OE1	2:B:217:GLN:N	2.44	0.47
1:A:76:LEU:HD22	1:A:500:PHE:HA	1.97	0.47
4:D:71:GLY:HA2	4:D:74:GLN:HB2	1.96	0.47
1:A:349:MET:HE1	1:A:395:VAL:HG23	1.96	0.47
1:A:63:SER:O	1:A:67:MET:HG2	2.14	0.47
1:E:32:PHE:HA	1:E:36:TYR:HB2	1.96	0.47
1:A:353:ILE:HB	1:A:354:PRO:HD3	1.96	0.47
1:A:68:LEU:HD22	5:A:1001:HEA:H262	1.97	0.47
2:B:210:ASN:O	2:B:213:VAL:HG12	2.15	0.47
2:B:272:SER:OG	2:B:273:PRO:HD3	2.13	0.47
1:E:166:TRP:H	5:E:1001:HEA:CGD	2.28	0.47
2:F:43:LEU:O	2:F:45:LYS:N	2.44	0.47
1:A:136:TYR:OH	1:A:588:ARG:HD3	2.14	0.47
3:C:86:HIS:HE1	3:C:96:VAL:HA	1.80	0.47
1:E:54:LYS:HZ1	1:E:544:PRO:HB2	1.79	0.47
1:A:187:LEU:HD23	1:A:250:SER:HA	1.97	0.47
1:A:412:LEU:CD1	5:A:1002:HEA:HHA	2.45	0.47
1:A:418:TYR:HA	1:A:460:PHE:HZ	1.80	0.47
1:A:68:LEU:O	1:A:72:GLY:N	2.48	0.47
3:C:187:VAL:HG13	4:D:58:GLN:HG3	1.97	0.47
1:E:239:PHE:H	1:E:240:PRO:CD	2.28	0.47
2:F:190:THR:HG21	1:E:99:PHE:HE1	1.79	0.47
1:E:607:TRP:CD1	1:E:611:GLY:HA2	2.49	0.47
1:E:204:PHE:HB2	1:E:232:MET:HG3	1.97	0.47
3:G:85:VAL:HA	3:G:89:ARG:HB2	1.97	0.47
1:A:178:SER:HB2	2:B:270:ALA:O	2.15	0.46
2:B:43:LEU:HD13	2:B:47:ARG:CZ	2.45	0.46
1:E:275:PHE:O	1:E:279:GLY:N	2.48	0.46
1:E:412:LEU:CD1	5:E:1002:HEA:HHA	2.45	0.46
1:E:92:SER:O	1:E:96:ASN:ND2	2.49	0.46
2:B:80:ILE:HA	2:B:83:SER:HB3	1.98	0.46
1:A:206:VAL:HG21	3:C:26:GLY:HA2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:148:ASP:N	2:F:148:ASP:OD1	2.48	0.46
3:C:75:LEU:HD21	3:C:182:TRP:HE1	1.81	0.46
1:E:444:LEU:HG	1:E:512:ASN:HB3	1.96	0.46
3:G:187:VAL:HG13	4:H:58:GLN:HB3	1.97	0.46
4:D:86:ILE:O	4:D:90:LEU:HB3	2.14	0.46
1:A:178:SER:OG	1:A:179:PRO:HD3	2.16	0.46
1:E:282:GLU:HA	1:E:285:ILE:HD12	1.96	0.46
2:F:101:LYS:HE2	2:F:103:LYS:HG2	1.96	0.46
1:E:353:ILE:HB	1:E:354:PRO:HD3	1.98	0.46
1:E:412:LEU:HD11	5:E:1002:HEA:HAD2	1.96	0.46
2:F:240:LEU:HD12	2:F:242:PHE:HE1	1.80	0.46
1:E:416:PHE:CE2	5:E:1001:HEA:HHD	2.50	0.46
3:G:188:VAL:HA	3:G:191:PHE:HB2	1.98	0.46
1:A:396:MET:O	1:A:406:TYR:OH	2.29	0.46
1:A:96:ASN:HA	1:A:99:PHE:HD1	1.80	0.46
2:B:191:GLY:O	2:B:193:HIS:N	2.49	0.46
1:E:283:VAL:HG13	5:E:1002:HEA:C3C	2.46	0.46
3:G:21:ARG:HD3	3:G:21:ARG:HA	1.66	0.46
1:A:416:PHE:CD1	5:A:1002:HEA:HMD3	2.51	0.46
2:B:114:ASP:O	2:B:116:LYS:N	2.47	0.46
2:B:127:GLU:CD	2:B:246:HIS:HD2	2.20	0.46
2:B:80:ILE:HD12	2:B:83:SER:HB3	1.96	0.46
3:C:73:LEU:HD11	4:D:57:LEU:HD21	1.98	0.46
1:E:385:PRO:O	1:E:389:ILE:HG13	2.16	0.46
1:E:432:PHE:HB3	1:E:433:ILE:HD12	1.98	0.45
1:E:45:SER:O	1:E:585:ASN:ND2	2.49	0.45
5:A:1001:HEA:HMC1	5:A:1001:HEA:HBC1	1.98	0.45
1:A:127:ILE:HG13	1:A:129:ALA:H	1.81	0.45
1:A:137:LEU:HD11	3:C:27:PHE:CZ	2.50	0.45
1:A:426:PHE:O	1:A:430:ALA:N	2.40	0.45
1:A:213:THR:OG1	1:A:552:LEU:HB2	2.15	0.45
3:C:188:VAL:HG23	3:C:189:TRP:HE3	1.80	0.45
1:A:21:VAL:HB	1:A:157:VAL:HG21	1.98	0.45
1:A:144:THR:HB	1:A:196:GLY:HA3	1.97	0.45
1:A:183:GLU:HB3	1:A:253:ARG:CZ	2.46	0.45
1:A:393:THR:HG21	1:A:468:TYR:CZ	2.51	0.45
1:E:106:MET:HB3	1:E:107:ILE:HD12	1.99	0.45
1:E:486:ASP:HB3	1:E:488:TRP:CE2	2.51	0.45
2:F:250:VAL:HG21	2:F:258:TYR:CD1	2.52	0.45
2:F:36:PHE:O	2:F:40:THR:OG1	2.23	0.45
2:B:112:SER:O	2:B:146:SER:OG	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:418:TYR:HA	1:E:460:PHE:HZ	1.81	0.45
2:F:120:SER:HA	2:F:127:GLU:HA	1.99	0.45
3:C:24:ILE:O	3:C:28:TRP:HB2	2.16	0.45
2:F:113:VAL:HA	2:F:147:ALA:HB3	1.97	0.45
1:E:326:VAL:HG22	1:E:329:HIS:ND1	2.29	0.45
1:E:446:GLU:O	1:E:450:LYS:HD3	2.17	0.45
1:E:620:LEU:O	1:E:624:LEU:HG	2.17	0.45
1:E:96:ASN:HA	1:E:99:PHE:CD1	2.51	0.45
1:A:24:ALA:O	1:A:28:ILE:HG12	2.17	0.45
3:C:73:LEU:HD23	4:D:10:UNK:HA	1.99	0.45
1:A:210:LYS:NZ	4:D:70:ASN:OD1	2.49	0.45
1:E:319:ILE:HG23	1:E:354:PRO:HB2	1.98	0.45
1:E:539:THR:HG21	1:E:544:PRO:CG	2.46	0.45
1:E:178:SER:OG	1:E:179:PRO:HD3	2.17	0.45
2:F:228:TYR:HD2	2:F:249:TYR:CD2	2.33	0.45
1:A:97:GLU:HA	1:A:162:PRO:O	2.17	0.44
1:A:466:PRO:O	1:A:470:LEU:N	2.40	0.44
1:A:60:TYR:HB3	1:A:113:PRO:O	2.17	0.44
2:B:224:THR:OG1	2:B:224:THR:O	2.31	0.44
1:E:134:PHE:O	1:E:203:ASN:ND2	2.47	0.44
1:A:212:ARG:NH1	1:A:218:LEU:HD12	2.32	0.44
3:C:83:ILE:HD13	3:C:176:PHE:HD1	1.82	0.44
4:H:59:LEU:O	4:H:63:MET:HB2	2.16	0.44
1:A:420:LEU:HD23	5:A:1001:HEA:HAC	1.99	0.44
1:A:283:VAL:HG13	5:A:1002:HEA:C3C	2.47	0.44
1:A:179:PRO:HG3	2:B:272:SER:HB3	1.98	0.44
1:A:534:THR:O	1:A:561:PHE:HB2	2.17	0.44
1:E:82:LEU:HD21	1:E:480:TYR:HA	1.99	0.44
1:E:90:LEU:HD13	1:E:98:ILE:HD12	1.98	0.44
3:C:141:LEU:HD21	3:C:192:ILE:HG21	2.00	0.44
3:C:191:PHE:HA	3:C:194:THR:HG22	1.99	0.44
4:D:67:GLU:HA	4:D:68:SER:HA	1.74	0.44
2:B:117:TRP:HB3	2:B:119:PHE:CE2	2.53	0.44
2:B:37:VAL:HG13	2:B:41:ILE:HD12	1.98	0.44
2:F:71:TRP:O	2:F:75:PRO:HD3	2.18	0.44
1:A:303:ARG:NH2	1:A:531:VAL:HG21	2.33	0.44
1:A:551:VAL:HG22	1:A:572:TYR:HD1	1.82	0.44
3:C:86:HIS:CE1	3:C:96:VAL:HA	2.52	0.44
1:E:61:ILE:HG13	1:E:62:ILE:N	2.33	0.44
1:A:234:ILE:HB	1:A:285:ILE:HG12	2.00	0.44
3:G:72:PHE:HA	3:G:75:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLY:HA3	2:B:162:LYS:HE3	1.99	0.44
1:A:588:ARG:HE	1:A:624:LEU:HB3	1.82	0.44
1:E:208:ILE:HD13	1:E:229:LEU:HB2	1.98	0.44
2:F:250:VAL:C	2:F:252:HIS:H	2.19	0.44
4:H:88:ILE:HG12	1:E:277:ILE:HD13	1.99	0.44
1:E:606:GLU:HB3	1:E:607:TRP:HE3	1.83	0.44
1:A:106:MET:HB3	1:A:107:ILE:HD12	1.99	0.43
1:A:194:GLY:O	1:A:198:LEU:HB2	2.18	0.43
2:F:125:ASP:HB3	2:F:244:SER:HA	2.00	0.43
2:F:210:ASN:N	2:F:210:ASN:HD22	2.15	0.43
3:G:96:VAL:HB	3:G:162:LEU:CD1	2.48	0.43
1:A:259:PHE:CE1	3:C:136:GLY:HA2	2.52	0.43
2:B:140:ILE:HD12	2:B:142:PHE:CZ	2.53	0.43
4:D:77:ASN:HA	4:D:80:PHE:CE1	2.53	0.43
3:G:187:VAL:HA	4:H:58:GLN:OE1	2.17	0.43
2:B:182:TYR:HB2	2:B:201:VAL:HG23	2.00	0.43
1:E:191:GLN:OE1	1:E:246:LEU:HB2	2.18	0.43
1:E:376:PRO:HB3	1:E:434:PHE:HB2	2.01	0.43
1:E:96:ASN:HA	1:E:99:PHE:HD1	1.84	0.43
2:F:115:TRP:CZ2	2:F:236:ASN:HA	2.53	0.43
1:A:156:PHE:HE1	7:A:1004:HQO:N1	2.16	0.43
1:A:326:VAL:HG22	1:A:329:HIS:CD2	2.46	0.43
1:A:607:TRP:HD1	1:A:611:GLY:HA2	1.82	0.43
2:B:113:VAL:HA	2:B:147:ALA:HB3	2.01	0.43
1:E:187:LEU:HD11	1:E:249:LEU:HD23	2.00	0.43
1:E:235:ILE:CG1	1:E:285:ILE:HD13	2.49	0.43
1:E:374:THR:O	1:E:378:LEU:HG	2.18	0.43
2:B:124:GLN:O	2:B:126:ILE:N	2.52	0.43
3:C:158:ILE:HD12	3:C:175:ILE:HA	2.00	0.43
2:F:111:THR:HG21	2:F:252:HIS:CD2	2.54	0.43
4:H:67:GLU:HA	4:H:68:SER:HA	1.73	0.43
1:A:416:PHE:CE1	5:A:1002:HEA:HMD3	2.53	0.43
1:A:73:VAL:O	1:A:77:MET:HG2	2.19	0.43
1:A:140:LEU:HD22	1:A:592:MET:SD	2.59	0.43
1:A:280:HIS:HA	1:A:283:VAL:HB	2.00	0.43
1:A:313:VAL:O	1:A:316:ILE:HG22	2.19	0.43
1:E:539:THR:OG1	1:E:541:SER:O	2.31	0.43
3:G:144:HIS:CE1	3:G:189:TRP:CD2	3.06	0.43
4:H:57:LEU:O	4:H:61:MET:HB2	2.18	0.43
1:A:244:VAL:HA	1:A:247:ALA:HB3	2.00	0.42
1:A:248:LEU:HD22	1:A:259:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:ARG:NE	1:A:624:LEU:HB3	2.34	0.42
1:A:257:ALA:HB2	3:C:128:LEU:HD13	2.00	0.42
2:F:142:PHE:HB3	2:F:144:ILE:HD11	2.01	0.42
2:F:144:ILE:HD12	2:F:153:LEU:HD21	2.00	0.42
1:A:19:ALA:O	1:A:23:ILE:HG13	2.18	0.42
3:G:25:LEU:HD12	1:E:206:VAL:HG13	2.01	0.42
1:E:473:GLN:HB3	1:E:488:TRP:CE2	2.53	0.42
1:A:258:HIS:CD2	3:C:129:SER:HA	2.55	0.42
2:B:175:GLN:HE21	2:B:176:ALA:H	1.67	0.42
1:E:304:LYS:HG2	1:E:305:GLN:H	1.83	0.42
1:E:238:ALA:HB2	1:E:324:PHE:CE2	2.54	0.42
1:E:416:PHE:CD1	5:E:1002:HEA:HMD3	2.54	0.42
4:H:57:LEU:HD22	4:H:58:GLN:HE22	1.84	0.42
1:A:140:LEU:HD11	1:A:199:MET:SD	2.59	0.42
1:A:305:GLN:O	1:A:307:PHE:N	2.53	0.42
1:E:416:PHE:HZ	5:E:1001:HEA:HHD	1.82	0.42
3:G:29:ILE:HA	4:H:77:ASN:OD1	2.18	0.42
1:A:106:MET:HG2	5:A:1001:HEA:C2C	2.49	0.42
1:A:412:LEU:HD13	5:A:1002:HEA:HBA1	2.01	0.42
2:B:97:PRO:HB2	2:B:98:GLU:H	1.57	0.42
1:E:412:LEU:HD11	5:E:1002:HEA:HHA	2.01	0.42
2:F:233:LEU:HD13	2:F:284:LYS:HZ3	1.83	0.42
1:A:231:THR:HG21	1:A:289:PRO:HG3	2.02	0.42
3:C:188:VAL:HG23	3:C:189:TRP:CE3	2.55	0.42
1:A:404:TYR:O	2:B:161:GLN:HG2	2.20	0.42
2:B:128:THR:HG22	2:B:129:VAL:H	1.85	0.42
2:B:152:SER:OG	2:B:187:ALA:HB2	2.19	0.42
2:B:154:TRP:HA	2:B:161:GLN:HB3	2.01	0.42
1:E:118:LEU:HD11	1:E:431:GLY:O	2.19	0.42
1:A:416:PHE:CZ	5:A:1001:HEA:HHD	2.55	0.42
1:E:144:THR:O	1:E:192:ILE:HG22	2.20	0.42
3:G:26:GLY:HA3	1:E:134:PHE:CZ	2.55	0.42
1:A:221:MET:N	1:A:222:PRO:HA	2.35	0.42
1:A:299:SER:O	1:A:533:ARG:HD3	2.20	0.42
1:E:123:VAL:HG21	1:E:228:THR:HG21	2.01	0.42
2:B:221:PRO:O	2:B:222:LYS:HG2	2.20	0.41
2:B:228:TYR:HD2	2:B:249:TYR:HD2	1.68	0.41
1:A:216:MET:HE3	1:A:555:VAL:HG11	2.02	0.41
1:E:195:ILE:HD13	1:E:195:ILE:HA	1.91	0.41
2:F:191:GLY:O	2:F:193:HIS:N	2.53	0.41
3:G:155:ILE:O	3:G:159:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:66:LEU:O	3:G:70:MET:HB2	2.20	0.41
1:A:188:LEU:O	1:A:192:ILE:HG13	2.20	0.41
1:A:204:PHE:CB	1:A:232:MET:HG3	2.50	0.41
2:B:101:LYS:HB2	2:B:101:LYS:HE3	1.88	0.41
1:E:465:PHE:HA	1:E:468:TYR:CD2	2.55	0.41
1:E:465:PHE:N	1:E:466:PRO:HD2	2.35	0.41
1:E:490:THR:HG23	1:E:491:LEU:HD22	2.01	0.41
2:B:233:LEU:HB2	2:B:284:LYS:NZ	2.35	0.41
2:F:74:ILE:N	2:F:75:PRO:CD	2.84	0.41
1:A:156:PHE:HE1	7:A:1004:HQO:C3	2.34	0.41
2:B:200:ASP:OD1	2:B:200:ASP:N	2.54	0.41
3:C:167:LEU:HD13	3:C:171:THR:HG22	2.01	0.41
1:E:367:TYR:C	1:E:369:GLY:H	2.23	0.41
1:A:231:THR:HG23	1:A:285:ILE:HG23	2.03	0.41
1:A:392:VAL:HB	2:B:29:LEU:HB3	2.03	0.41
1:A:416:PHE:HZ	5:A:1001:HEA:HHD	1.86	0.41
3:C:83:ILE:HA	3:C:86:HIS:HB3	2.02	0.41
3:G:27:PHE:O	3:G:31:LEU:HG	2.20	0.41
1:A:466:PRO:HG3	1:A:494:ILE:HG22	2.02	0.41
2:B:27:PHE:HA	2:B:30:PHE:HB2	2.02	0.41
3:C:45:PHE:CE2	3:C:196:VAL:HG12	2.56	0.41
1:E:116:ILE:O	1:E:120:ASN:N	2.38	0.41
1:E:574:GLU:HG3	1:E:577:PHE:CE2	2.56	0.41
1:E:97:GLU:HA	1:E:162:PRO:O	2.20	0.41
3:G:61:LEU:HD12	3:G:64:VAL:HG23	2.03	0.41
3:C:141:LEU:CA	3:C:144:HIS:HB3	2.50	0.41
1:E:298:ILE:HG21	1:E:362:TRP:CD1	2.56	0.41
3:G:79:PHE:CE2	3:G:179:SER:HA	2.50	0.41
1:A:115:LEU:HA	1:A:115:LEU:HD12	1.80	0.41
1:A:318:ALA:HB3	1:A:354:PRO:HB3	2.03	0.41
1:A:310:LYS:HE2	2:B:65:THR:HG23	2.02	0.41
1:E:170:MET:N	1:E:171:PRO:HD2	2.36	0.41
2:F:250:VAL:O	2:F:252:HIS:N	2.45	0.41
2:F:276:LYS:HB3	2:F:277:THR:H	1.72	0.41
3:G:180:LEU:HD11	4:H:65:MET:HB2	2.01	0.41
1:A:305:GLN:O	1:A:365:THR:HG23	2.21	0.41
3:C:55:GLY:C	2:F:225:LYS:HE3	2.41	0.41
1:E:313:VAL:O	1:E:316:ILE:HG22	2.21	0.41
2:F:149:SER:HB3	1:E:176:ASP:OD2	2.21	0.41
3:G:104:LEU:HD11	3:G:152:ILE:HG23	2.02	0.41
3:G:155:ILE:O	3:G:158:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:PHE:CD1	5:A:1001:HEA:H261	2.55	0.40
1:A:170:MET:N	1:A:171:PRO:HD2	2.36	0.40
1:A:79:ARG:NH2	1:A:495:SER:HB3	2.28	0.40
1:A:334:MET:HB3	2:B:163:TYR:CD2	2.56	0.40
3:G:180:LEU:HD11	4:H:65:MET:HG3	2.03	0.40
4:H:68:SER:OG	4:H:69:GLU:N	2.54	0.40
2:B:100:THR:HG23	2:B:101:LYS:H	1.87	0.40
1:E:190:LEU:HB2	1:E:246:LEU:HD11	2.04	0.40
2:F:163:TYR:HB2	1:E:334:MET:HA	2.04	0.40
1:A:202:ILE:HD13	3:C:30:PHE:HB2	2.03	0.40
1:A:465:PHE:N	1:A:466:PRO:HD2	2.36	0.40
1:E:82:LEU:HD11	1:E:95:TYR:OH	2.20	0.40
2:F:228:TYR:CD2	2:F:249:TYR:HD2	2.34	0.40
2:F:74:ILE:O	2:F:78:ILE:HG12	2.21	0.40
3:G:68:MET:HB3	3:G:110:PHE:CE1	2.57	0.40
3:G:85:VAL:HG13	3:G:89:ARG:HD2	2.02	0.40
2:F:106:LEU:HD23	2:F:140:ILE:HG22	2.04	0.40
1:A:54:LYS:HZ1	1:A:548:ASN:HB3	1.84	0.40
1:E:306:LEU:HD23	1:E:365:THR:HG21	2.03	0.40
2:F:80:ILE:HA	2:F:80:ILE:HD12	1.95	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	603/655 (92%)	509 (84%)	76 (13%)	18 (3%)	4	34
1	E	603/655 (92%)	510 (85%)	77 (13%)	16 (3%)	5	35
2	B	250/296 (84%)	188 (75%)	49 (20%)	13 (5%)	2	23
2	F	250/296 (84%)	189 (76%)	48 (19%)	13 (5%)	2	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	176/204 (86%)	154 (88%)	21 (12%)	1 (1%)	25	61
3	G	176/204 (86%)	157 (89%)	19 (11%)	0	100	100
4	D	46/124 (37%)	37 (80%)	7 (15%)	2 (4%)	2	26
4	H	46/124 (37%)	37 (80%)	7 (15%)	2 (4%)	2	26
All	All	2150/2558 (84%)	1781 (83%)	304 (14%)	65 (3%)	4	34

All (65) 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	98	GLU
2	B	279	PRO
2	F	97	PRO
2	F	98	GLU
2	F	125	ASP
1	E	178	SER
1	E	222	PRO
1	E	239	PHE
1	E	548	ASN
1	A	306	LEU
1	A	338	ALA
1	A	555	VAL
2	B	97	PRO
2	B	125	ASP
2	B	192	GLU
4	H	69	GLU
2	F	192	GLU
2	F	279	PRO
1	E	48	ILE
1	E	306	LEU
1	E	555	VAL
1	A	48	ILE
1	A	410	TYR
1	A	570	GLU
1	A	583	PRO
2	B	100	THR
2	B	273	PRO
2	F	273	PRO

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Mol	Chain	Res	Type
2	F	281	GLU
2	F	283	VAL
1	E	221	MET
1	E	338	ALA
1	E	410	TYR
1	E	570	GLU
1	E	583	PRO
1	A	95	TYR
1	A	221	MET
1	A	474	GLY
2	B	84	VAL
2	B	242	PHE
3	C	124	GLU
4	D	69	GLU
4	H	72	THR
2	F	240	LEU
2	F	242	PHE
1	E	95	TYR
1	E	216	MET
1	A	130	ARG
1	A	216	MET
2	B	281	GLU
2	B	283	VAL
4	D	72	THR
2	F	84	VAL
2	F	100	THR
1	E	474	GLY
2	B	177	ASP
2	B	278	ASP
2	F	278	ASP
1	A	326	VAL
1	A	385	PRO
1	E	385	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	512/558 (92%)	481 (94%)	31 (6%)	18	51
1	E	512/558 (92%)	477 (93%)	35 (7%)	16	47
2	B	230/263 (88%)	210 (91%)	20 (9%)	10	39
2	F	230/263 (88%)	207 (90%)	23 (10%)	7	32
3	C	151/171 (88%)	139 (92%)	12 (8%)	12	43
3	G	151/171 (88%)	141 (93%)	10 (7%)	16	48
4	D	38/59 (64%)	35 (92%)	3 (8%)	12	43
4	H	38/59 (64%)	36 (95%)	2 (5%)	22	54
All	All	1862/2102 (89%)	1726 (93%)	136 (7%)	14	45

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	TYR
1	A	70	ARG
1	A	93	ASN
1	A	97	GLU
1	A	99	PHE
1	A	106	MET
1	A	114	PHE
1	A	115	LEU
1	A	139	ASN
1	A	145	PHE
1	A	151	LEU
1	A	172	LEU
1	A	177	MET
1	A	210	LYS
1	A	216	MET
1	A	239	PHE
1	A	251	PHE
1	A	260	PHE
1	A	273	ASN
1	A	288	LEU
1	A	310	LYS
1	A	363	LEU
1	A	395	VAL
1	A	416	PHE
1	A	432	PHE
1	A	436	TYR
1	A	500	PHE

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Mol	Chain	Res	Type
1	A	552	LEU
1	A	571	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	115	TRP
2	B	153	LEU
2	B	165	MET
2	B	175	GLN
2	B	188	ASN
2	B	213	VAL
2	B	224	THR
2	B	228	TYR
2	B	232	MET
2	B	237	VAL
2	B	252	HIS
2	B	258	TYR
2	B	268	TYR
2	B	272	SER
2	B	277	THR
2	B	284	LYS
3	C	25	LEU
3	C	56	VAL
3	C	59	ASP
3	C	61	LEU
3	C	72	PHE
3	C	75	LEU
3	C	79	PHE
3	C	93	LEU
3	C	128	LEU
3	C	161	GLN
3	C	189	TRP
3	C	192	ILE
4	D	62	PHE
4	D	69	GLU
4	D	80	PHE
3	G	22	LEU
3	G	61	LEU
3	G	72	PHE

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Mol	Chain	Res	Type
3	G	75	LEU
3	G	79	PHE
3	G	93	LEU
3	G	97	VAL
3	G	128	LEU
3	G	161	GLN
3	G	189	TRP
4	H	69	GLU
4	H	79	LEU
2	F	22	LEU
2	F	28	MET
2	F	29	LEU
2	F	39	PHE
2	F	100	THR
2	F	102	ASP
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	215	LYS
2	F	223	LEU
2	F	224	THR
2	F	228	TYR
2	F	232	MET
2	F	237	VAL
2	F	246	HIS
2	F	252	HIS
2	F	277	THR
2	F	283	VAL
1	E	36	TYR
1	E	70	ARG
1	E	79	ARG
1	E	93	ASN
1	E	96	ASN
1	E	97	GLU
1	E	99	PHE
1	E	104	THR
1	E	105	ILE
1	E	106	MET

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Mol	Chain	Res	Type
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	177	MET
1	E	187	LEU
1	E	210	LYS
1	E	216	MET
1	E	239	PHE
1	E	260	PHE
1	E	273	ASN
1	E	310	LYS
1	E	363	LEU
1	E	395	VAL
1	E	415	HIS
1	E	416	PHE
1	E	432	PHE
1	E	436	TYR
1	E	500	PHE
1	E	581	HIS
1	E	633	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	329	HIS
2	B	175	GLN
2	B	246	HIS
2	B	252	HIS
4	H	58	GLN
2	F	210	ASN
2	F	252	HIS
1	E	184	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	1002	-	44,67,67	1.88	10 (22%)	37,103,103	2.48	14 (37%)
5	HEA	E	1002	1	44,67,67	1.87	10 (22%)	37,103,103	2.41	13 (35%)
7	HQO	A	1004	1	14,14,20	3.23	3 (21%)	13,20,26	1.43	1 (7%)
5	HEA	A	1001	1	44,67,67	1.99	11 (25%)	37,103,103	2.17	10 (27%)
5	HEA	E	1001	1	44,67,67	1.97	11 (25%)	37,103,103	2.00	8 (21%)
7	HQO	E	1004	-	14,14,20	3.20	3 (21%)	13,20,26	1.49	1 (7%)

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	A	1002	-	2/2/7/16	1/24/76/76	-
5	HEA	E	1002	1	2/2/7/16	1/24/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HQO	A	1004	1	-	-	0/2/2/2
5	HEA	A	1001	1	2/2/7/16	5/24/76/76	-
5	HEA	E	1001	1	2/2/7/16	5/24/76/76	-
7	HQO	E	1004	-	-	-	0/2/2/2

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1004	HQO	O4-N1	-10.62	1.24	1.38
7	E	1004	HQO	O4-N1	-10.52	1.24	1.38
5	E	1001	HEA	C3A-C2A	6.56	1.49	1.40
5	A	1001	HEA	C3A-C2A	6.18	1.49	1.40
5	A	1002	HEA	C3B-C11	-6.17	1.48	1.52
5	E	1002	HEA	C3B-C11	-5.70	1.48	1.52
5	E	1002	HEA	C3A-C2A	5.58	1.48	1.40
5	A	1001	HEA	C3B-C11	-5.57	1.48	1.52
5	A	1001	HEA	C3C-C2C	5.42	1.47	1.40
5	E	1001	HEA	C3C-C2C	5.38	1.47	1.40
5	A	1002	HEA	C3A-C2A	5.30	1.47	1.40
5	E	1002	HEA	C3C-C2C	5.15	1.47	1.40
5	A	1002	HEA	C3C-C2C	5.11	1.47	1.40
5	E	1001	HEA	C3B-C11	-4.63	1.49	1.52
5	E	1001	HEA	C1A-C2A	3.60	1.50	1.42
5	A	1001	HEA	C3D-C2D	3.51	1.48	1.37
7	E	1004	HQO	C10-C5	3.50	1.48	1.42
5	E	1001	HEA	C3D-C2D	3.46	1.47	1.37
7	A	1004	HQO	C10-C5	3.46	1.48	1.42
5	A	1001	HEA	C1A-C2A	3.44	1.50	1.42
5	E	1002	HEA	C3D-C2D	3.32	1.47	1.37
7	E	1004	HQO	C1-C10	3.25	1.48	1.42
7	A	1004	HQO	C1-C10	3.24	1.48	1.42
5	A	1002	HEA	C3D-C2D	3.22	1.47	1.37
5	A	1002	HEA	C1A-C2A	3.11	1.49	1.42
5	A	1002	HEA	C4B-C3B	3.07	1.49	1.42
5	E	1002	HEA	C1A-C2A	3.02	1.49	1.42
5	E	1001	HEA	C4B-C3B	3.01	1.49	1.42
5	A	1001	HEA	C4B-C3B	3.01	1.49	1.42
5	E	1002	HEA	C4B-C3B	2.99	1.49	1.42
5	E	1001	HEA	C1D-C2D	2.96	1.49	1.42
5	E	1002	HEA	C1D-C2D	2.93	1.49	1.42
5	A	1001	HEA	C1D-C2D	2.90	1.49	1.42
5	A	1002	HEA	C1D-C2D	2.86	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	HEA	C1B-CHB	2.59	1.48	1.41
5	A	1001	HEA	C4C-CHD	2.58	1.48	1.41
5	E	1001	HEA	C1B-CHB	2.55	1.48	1.41
5	A	1001	HEA	C1C-CHC	2.45	1.47	1.41
5	E	1001	HEA	C4C-CHD	2.41	1.47	1.41
5	E	1001	HEA	C1C-CHC	2.36	1.47	1.41
5	E	1002	HEA	C4C-CHD	2.35	1.47	1.41
5	A	1001	HEA	C4D-CHA	2.34	1.47	1.41
5	A	1002	HEA	C1C-CHC	2.33	1.47	1.41
5	E	1001	HEA	C4D-CHA	2.27	1.47	1.41
5	A	1002	HEA	C4C-CHD	2.21	1.47	1.41
5	E	1002	HEA	C1C-CHC	2.20	1.47	1.41
5	A	1002	HEA	C1B-CHB	2.17	1.47	1.41
5	E	1002	HEA	C1B-CHB	2.06	1.46	1.41

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1002	HEA	C1B-C2B-C3B	-7.47	101.80	107.00
5	A	1002	HEA	C1B-C2B-C3B	-7.29	101.92	107.00
5	E	1001	HEA	C4B-C3B-C2B	-7.14	101.88	106.87
5	A	1001	HEA	C4B-C3B-C2B	-6.38	102.41	106.87
5	E	1002	HEA	C4B-C3B-C2B	-6.24	102.51	106.87
5	A	1002	HEA	C4B-C3B-C2B	-5.75	102.85	106.87
5	A	1001	HEA	C1B-C2B-C3B	-5.71	103.03	107.00
5	E	1001	HEA	C1B-C2B-C3B	-4.86	103.61	107.00
5	A	1002	HEA	C3C-C4C-NC	4.27	114.72	109.21
5	E	1002	HEA	C3C-C4C-NC	3.95	114.31	109.21
5	E	1002	HEA	CMC-C2C-C3C	3.91	132.00	124.68
5	A	1001	HEA	CMC-C2C-C3C	3.78	131.76	124.68
5	E	1001	HEA	C3C-C4C-NC	3.75	114.06	109.21
7	E	1004	HQO	O1-C1-C10	3.67	120.89	116.31
5	A	1002	HEA	CMC-C2C-C3C	3.66	131.52	124.68
5	A	1002	HEA	C13-C12-C11	-3.61	108.92	114.35
7	A	1004	HQO	O1-C1-C10	3.60	120.80	116.31
5	A	1001	HEA	C3C-C4C-NC	3.50	113.73	109.21
5	A	1002	HEA	C26-C15-C16	3.49	121.13	115.27
5	A	1002	HEA	C13-C14-C15	-3.45	119.36	127.66
5	E	1001	HEA	CMC-C2C-C3C	3.43	131.10	124.68
5	E	1002	HEA	C13-C14-C15	-3.32	119.66	127.66
5	E	1002	HEA	C26-C15-C16	3.22	120.69	115.27
5	A	1002	HEA	C27-C19-C20	3.15	120.56	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	HEA	C26-C15-C16	3.12	120.53	115.27
5	A	1001	HEA	C17-C18-C19	-2.88	120.73	127.66
5	E	1002	HEA	C17-C18-C19	-2.87	120.76	127.66
5	A	1002	HEA	C17-C18-C19	-2.86	120.77	127.66
5	E	1001	HEA	C26-C15-C16	2.71	119.83	115.27
5	A	1002	HEA	C25-C23-C24	2.68	120.52	114.60
5	E	1001	HEA	C27-C19-C20	2.57	119.60	115.27
5	A	1001	HEA	C27-C19-C20	2.56	119.58	115.27
5	A	1001	HEA	C25-C23-C24	2.49	120.09	114.60
5	E	1002	HEA	CBA-CAA-C2A	-2.47	107.93	112.48
5	E	1002	HEA	C25-C23-C24	2.46	120.03	114.60
5	A	1001	HEA	C13-C14-C15	-2.43	121.81	127.66
5	E	1002	HEA	C27-C19-C20	2.38	119.28	115.27
5	E	1002	HEA	C13-C12-C11	-2.28	110.93	114.35
5	E	1001	HEA	C17-C18-C19	-2.27	122.20	127.66
5	A	1002	HEA	CAD-CBD-CGD	-2.17	109.03	112.67
5	E	1002	HEA	CMB-C2B-C3B	2.14	128.87	124.69
5	A	1002	HEA	C21-C22-C23	-2.10	120.56	127.75
5	A	1002	HEA	CMB-C2B-C3B	2.10	128.80	124.69
5	A	1001	HEA	C13-C12-C11	-2.09	111.21	114.35
5	E	1002	HEA	C21-C22-C23	-2.09	120.62	127.75
5	E	1001	HEA	C25-C23-C24	2.06	119.16	114.60
5	A	1002	HEA	CMD-C2D-C3D	2.06	128.82	124.94

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1002	HEA	ND
5	A	1002	HEA	NB
5	E	1002	HEA	ND
5	E	1002	HEA	NB
5	A	1001	HEA	ND
5	A	1001	HEA	NB
5	E	1001	HEA	ND
5	E	1001	HEA	NB

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	HEA	C3B-C11-C12-C13
5	E	1001	HEA	C3B-C11-C12-C13
5	A	1001	HEA	C15-C16-C17-C18

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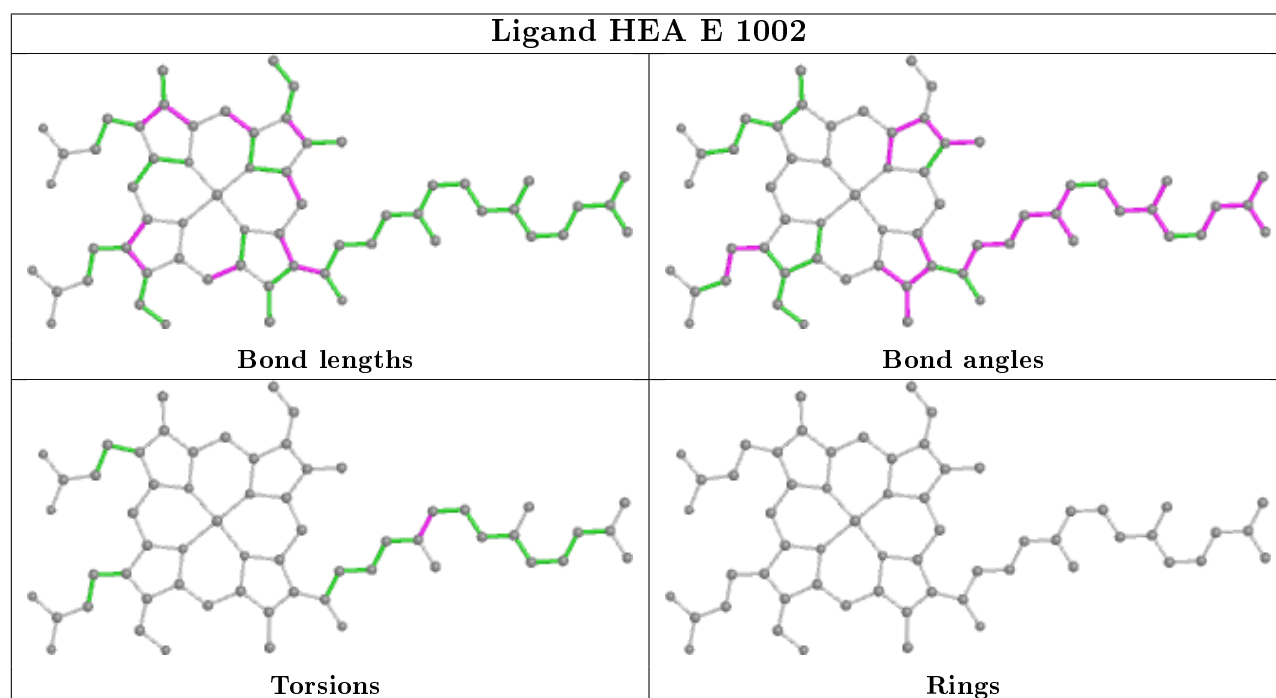
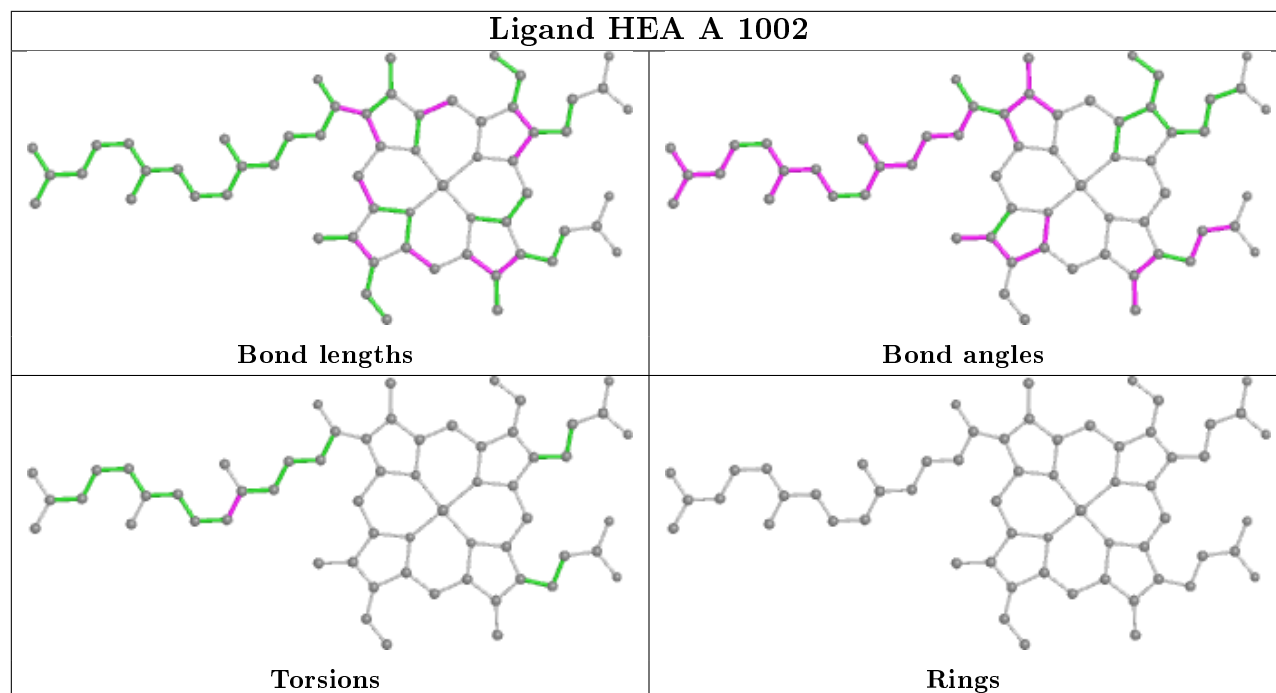
Mol	Chain	Res	Type	Atoms
5	E	1001	HEA	C15-C16-C17-C18
5	A	1001	HEA	C26-C15-C16-C17
5	E	1001	HEA	C26-C15-C16-C17
5	A	1001	HEA	C14-C15-C16-C17
5	E	1001	HEA	C14-C15-C16-C17
5	A	1001	HEA	O11-C11-C12-C13
5	E	1001	HEA	O11-C11-C12-C13
5	A	1002	HEA	C26-C15-C16-C17
5	E	1002	HEA	C26-C15-C16-C17

There are no ring outliers.

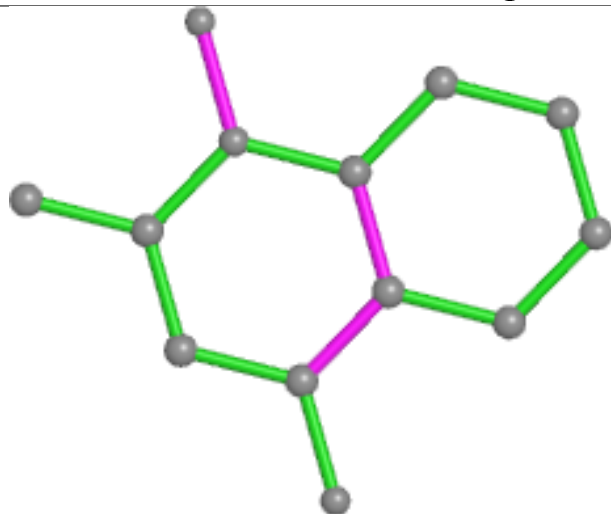
6 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1002	HEA	7	0
5	E	1002	HEA	7	0
7	A	1004	HQO	4	0
5	A	1001	HEA	11	0
5	E	1001	HEA	5	0
7	E	1004	HQO	5	0

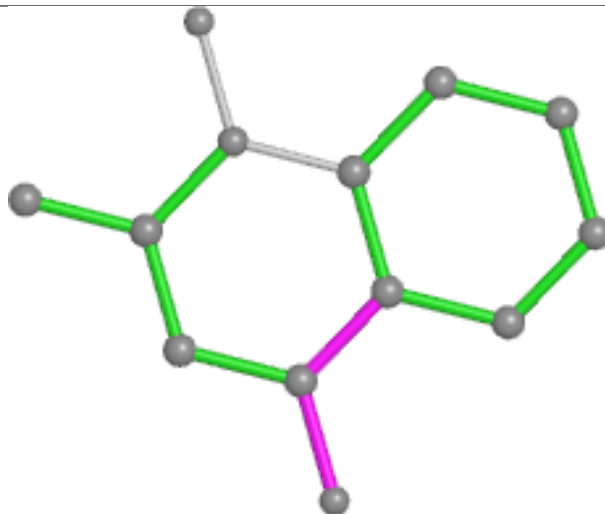
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



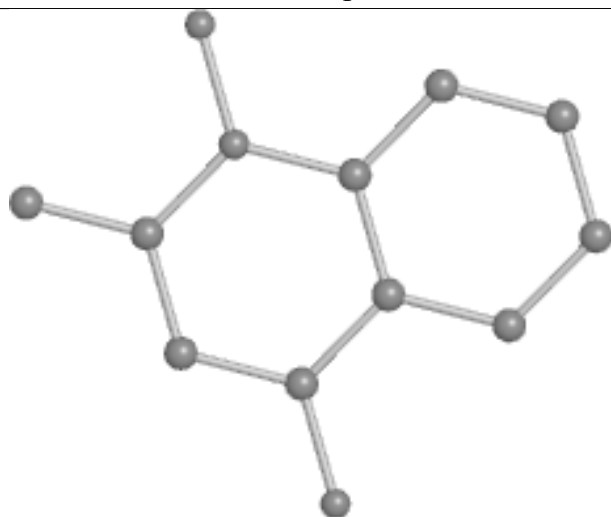
Ligand HQO A 1004



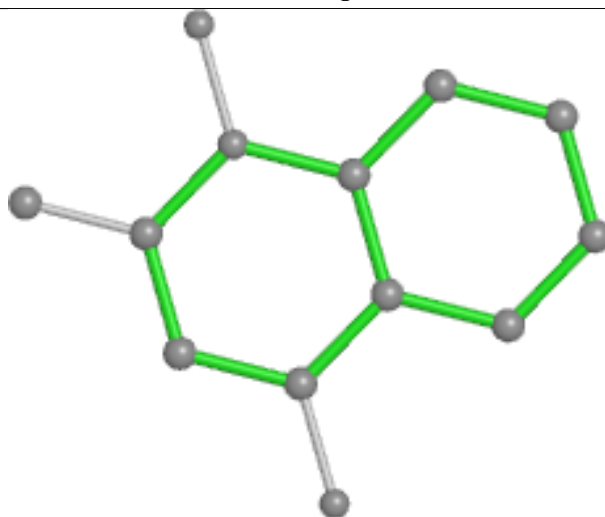
Bond lengths



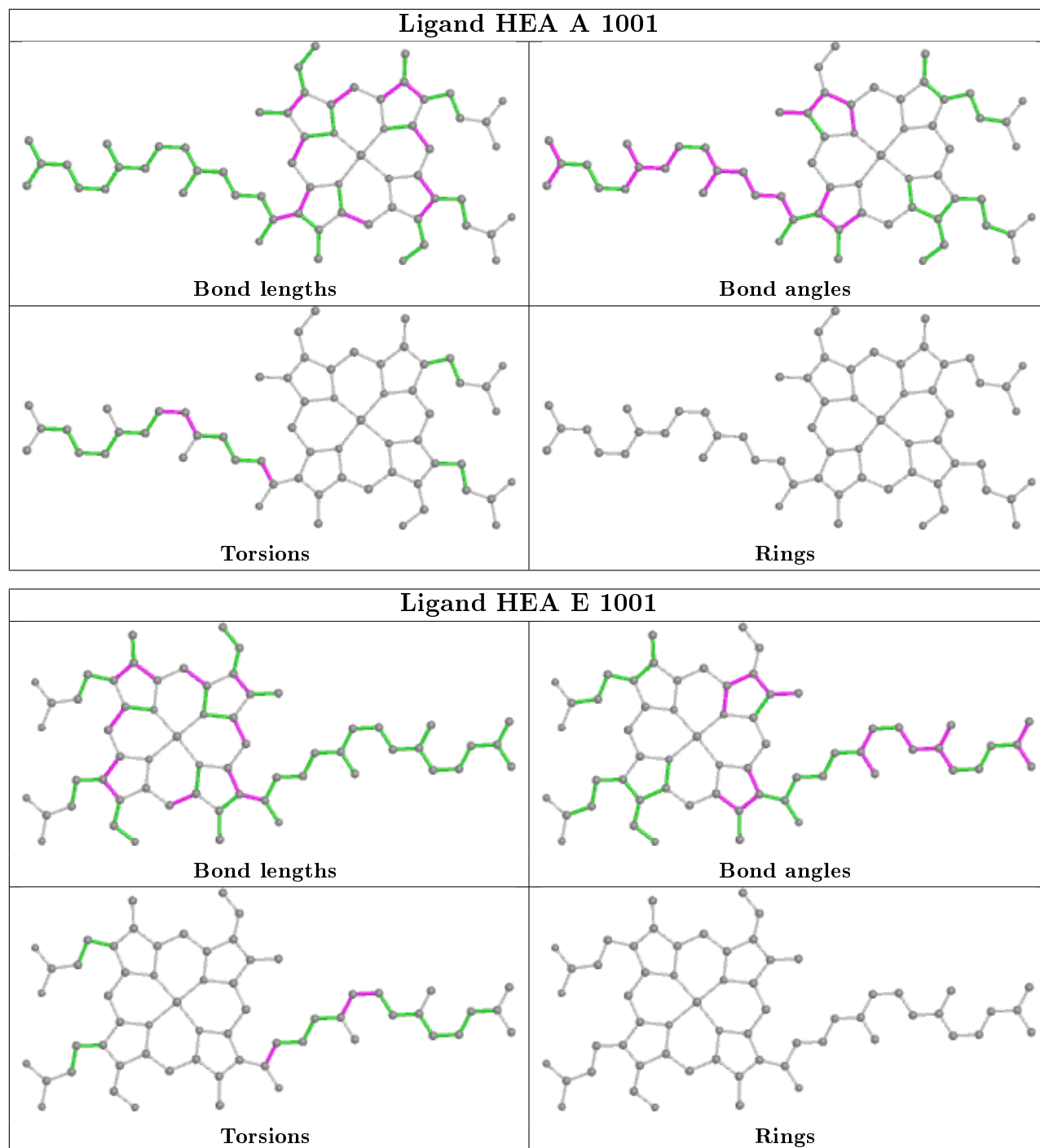
Bond angles

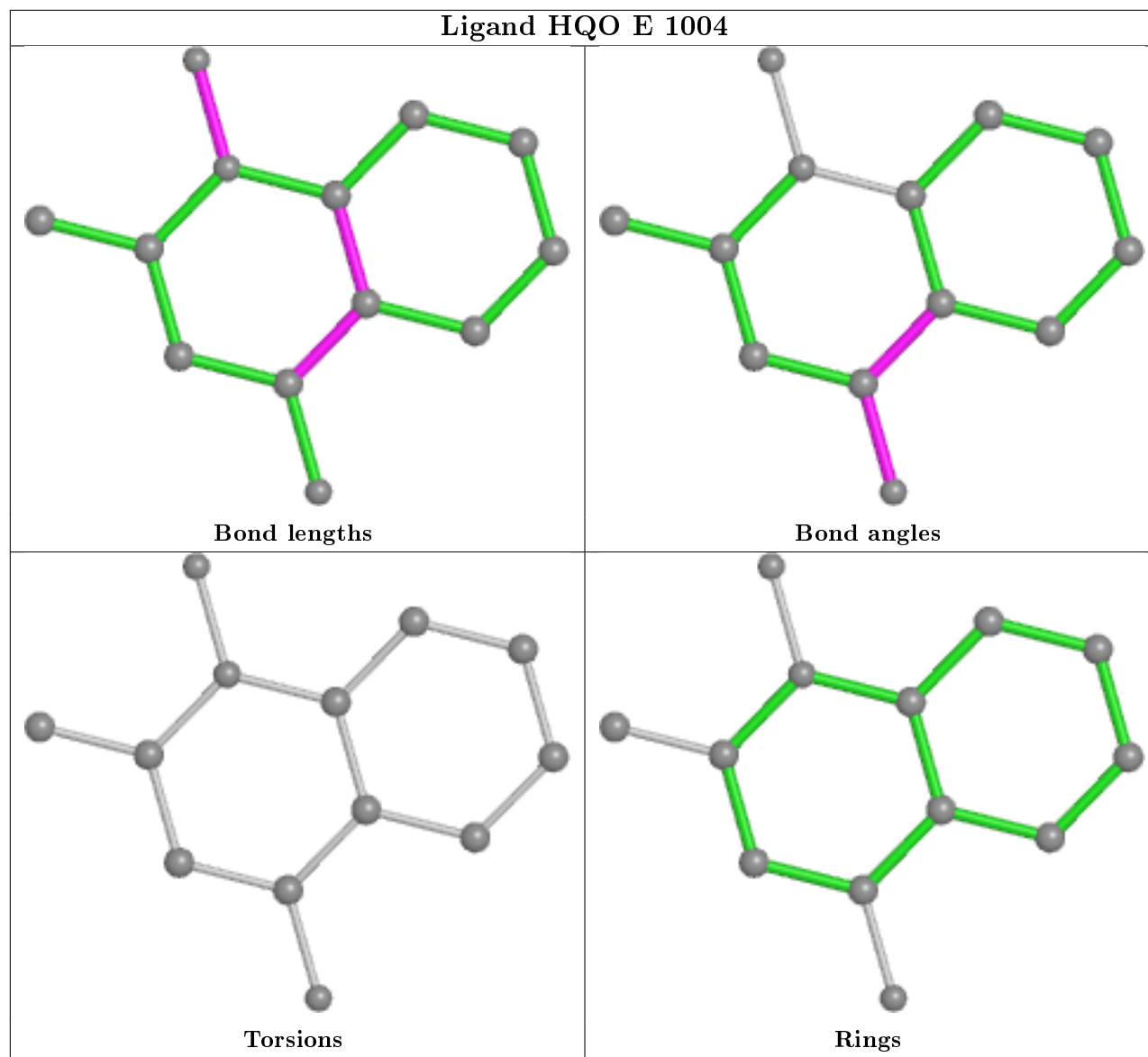


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	607/655 (92%)	0.02	13 (2%) 63 58	68, 108, 149, 180	0
1	E	607/655 (92%)	0.03	20 (3%) 46 40	66, 111, 155, 191	0
2	B	256/296 (86%)	0.44	31 (12%) 4 4	90, 139, 195, 223	0
2	F	256/296 (86%)	0.41	22 (8%) 10 9	79, 134, 197, 235	0
3	C	178/204 (87%)	-0.03	9 (5%) 28 25	79, 115, 191, 235	0
3	G	178/204 (87%)	0.03	12 (6%) 17 14	72, 124, 187, 200	0
4	D	48/124 (38%)	0.43	6 (12%) 3 4	81, 115, 158, 166	0
4	H	48/124 (38%)	-0.37	0 100 100	72, 109, 152, 160	0
All	All	2178/2558 (85%)	0.11	113 (5%) 27 25	66, 117, 179, 235	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	274	HIS	7.3
4	D	60	LEU	7.0
3	G	53	ALA	6.9
2	F	106	LEU	6.4
2	B	42	ILE	5.7
1	E	580	ILE	5.5
2	F	236	ASN	5.3
2	B	73	VAL	5.3
2	B	92	SER	5.2
2	B	95	LYS	5.0
2	F	288	PHE	4.9
2	B	236	ASN	4.4
1	E	370	ARG	4.3
3	C	80	THR	4.2
4	D	63	MET	4.1
2	F	135	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	86	ASN	4.0
1	A	441	GLY	4.0
3	C	97	VAL	3.9
2	F	27	PHE	3.9
3	G	57	LEU	3.8
1	A	14	PRO	3.8
3	G	52	THR	3.7
2	B	98	GLU	3.6
4	D	59	LEU	3.5
1	E	33	VAL	3.5
3	G	126	ALA	3.4
3	G	89	ARG	3.3
2	F	107	VAL	3.3
2	B	38	LEU	3.2
4	D	69	GLU	3.2
2	B	288	PHE	3.2
2	B	97	PRO	3.1
2	B	282	ASN	3.1
1	A	550	ALA	3.1
1	E	586	SER	3.0
1	A	541	SER	3.0
3	G	90	ARG	3.0
2	B	201	VAL	2.9
2	B	287	GLU	2.9
1	E	516	SER	2.9
1	E	441	GLY	2.9
2	F	277	THR	2.9
1	A	579	LYS	2.9
2	F	143	LYS	2.9
2	B	202	ASN	2.9
1	A	578	LYS	2.9
1	E	279	GLY	2.8
1	A	486	ASP	2.8
1	A	437	PRO	2.8
3	G	124	GLU	2.7
2	B	94	GLU	2.7
3	G	144	HIS	2.7
2	F	78	ILE	2.7
1	E	130	ARG	2.7
2	B	70	VAL	2.7
1	A	448	ILE	2.7
1	E	305	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	115	TRP	2.6
3	C	77	SER	2.6
2	B	191	GLY	2.6
2	B	34	VAL	2.6
2	B	41	ILE	2.6
2	F	134	ILE	2.6
2	B	16	GLN	2.6
1	A	540	SER	2.6
2	B	39	PHE	2.6
1	E	587	GLY	2.6
1	E	485	ASN	2.5
2	F	274	HIS	2.5
4	D	64	HIS	2.5
2	B	120	SER	2.5
3	G	54	GLY	2.5
1	E	584	SER	2.5
2	F	50	LYS	2.5
2	B	273	PRO	2.5
3	C	163	LYS	2.4
2	B	238	ASP	2.4
2	F	109	TYR	2.4
4	D	74	GLN	2.4
3	C	20	GLY	2.4
3	G	56	VAL	2.3
3	G	50	ASN	2.3
2	B	99	ALA	2.3
2	F	179	VAL	2.3
1	E	631	ASN	2.3
2	B	17	GLN	2.3
3	C	102	ILE	2.2
1	E	283	VAL	2.2
1	E	333	THR	2.2
2	F	251	ASP	2.2
1	A	48	ILE	2.2
3	C	61	LEU	2.2
1	A	46	GLU	2.1
1	E	583	PRO	2.1
2	B	102	ASP	2.1
2	B	132	LEU	2.1
1	E	34	LEU	2.1
2	F	28	MET	2.1
3	G	58	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	211	MET	2.1
3	C	50	ASN	2.1
2	B	45	LYS	2.1
3	C	81	CYS	2.1
2	F	158	LEU	2.1
1	E	478	ARG	2.1
2	F	287	GLU	2.1
1	E	280	HIS	2.0
2	B	108	VAL	2.0
2	B	131	TYR	2.0
2	F	49	ARG	2.0
2	F	16	GLN	2.0
2	F	211	SER	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 carbohydrates 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.

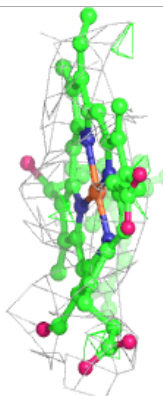
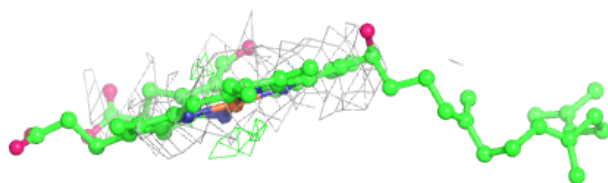
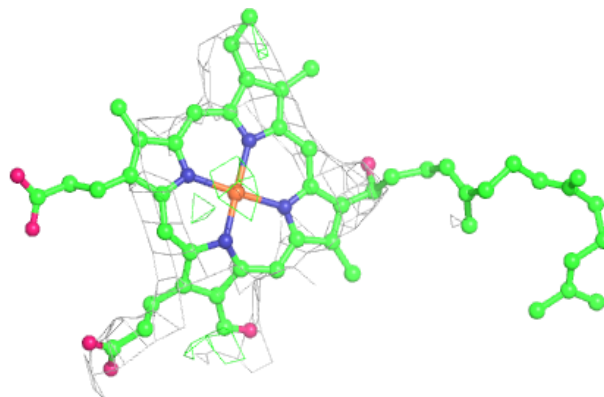
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	HEA	A	1002	60/60	0.73	0.48	96,118,163,168	0
5	HEA	E	1002	60/60	0.73	0.47	92,117,141,142	0
5	HEA	E	1001	60/60	0.78	0.50	88,109,131,135	0
6	CU	E	1003	1/1	0.79	0.29	104,104,104,104	0
5	HEA	A	1001	60/60	0.84	0.41	91,112,132,134	0
7	HQO	E	1004	13/19	0.84	0.22	102,107,111,114	0
6	CU	A	1003	1/1	0.85	0.20	109,109,109,109	0
7	HQO	A	1004	13/19	0.89	0.17	95,102,107,110	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.

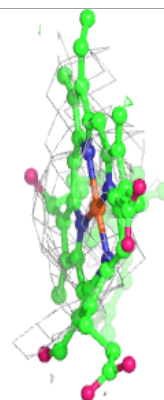
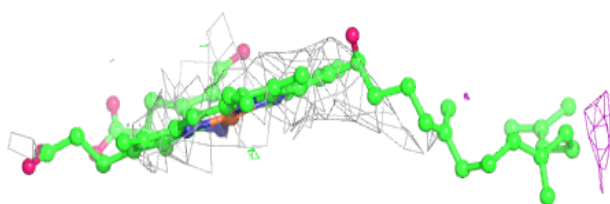
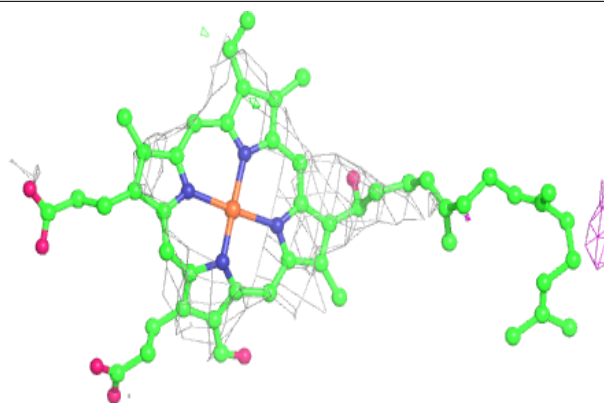
Electron density around HEA A 1002:

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

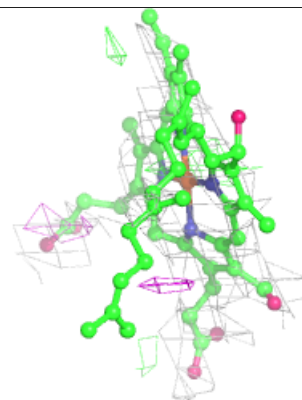
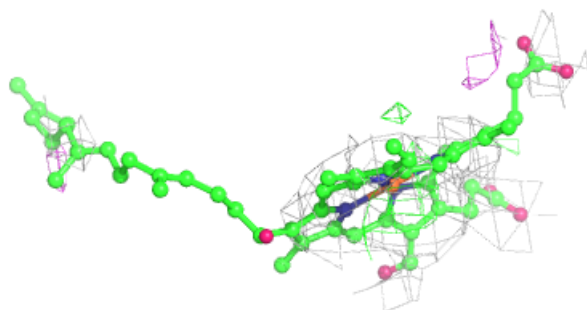
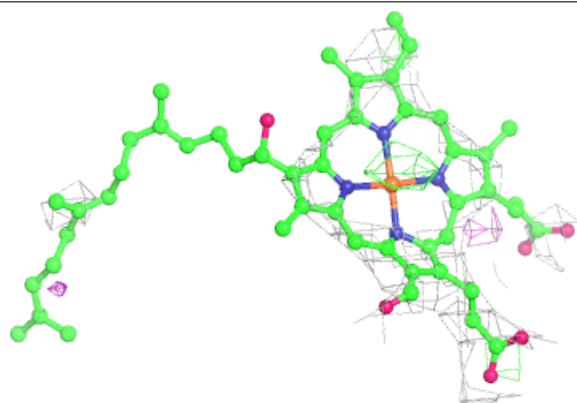


Electron density around HEA E 1002:

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

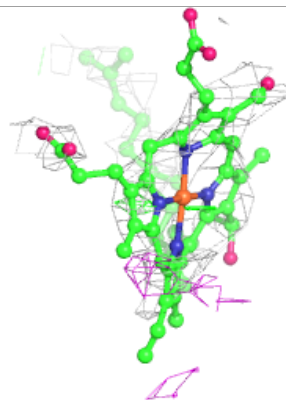
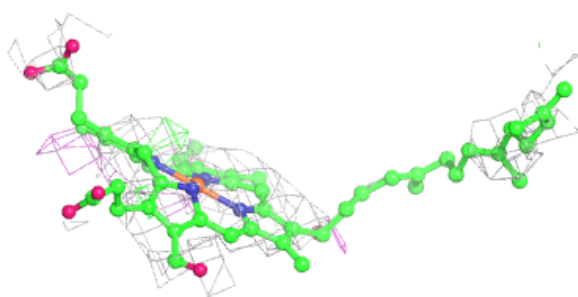
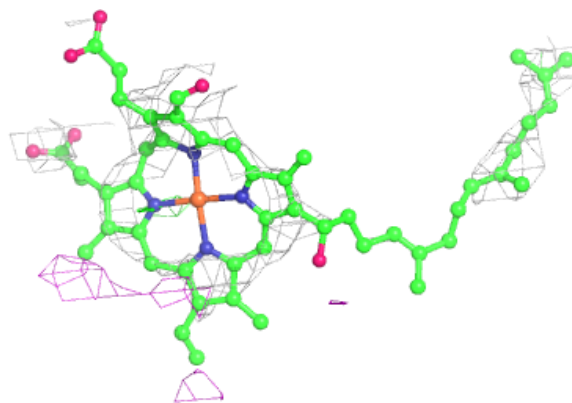
**Electron density around HEA E 1001:**

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



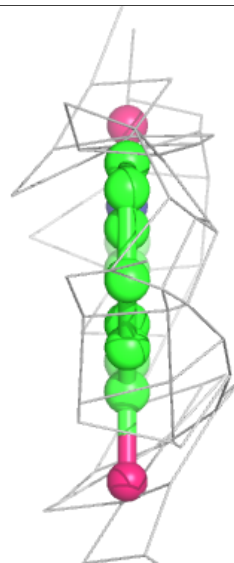
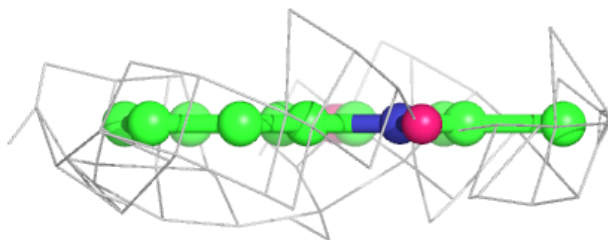
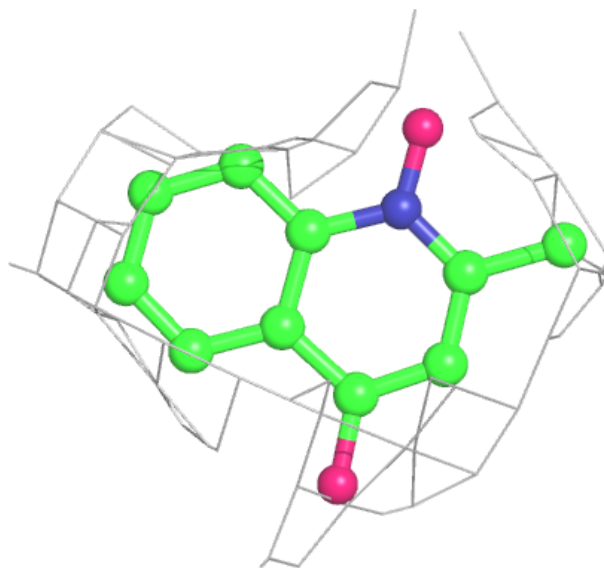
Electron density around HEA A 1001:

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



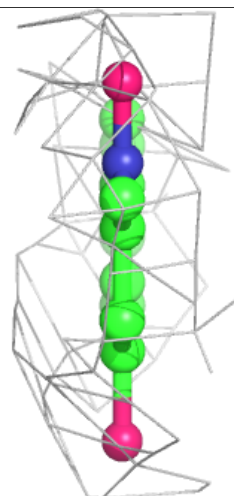
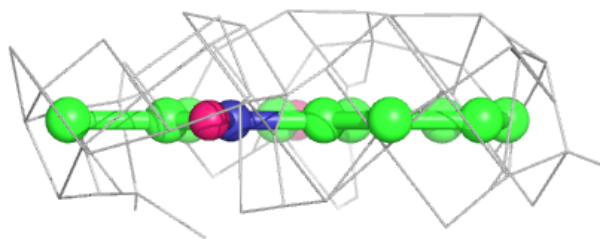
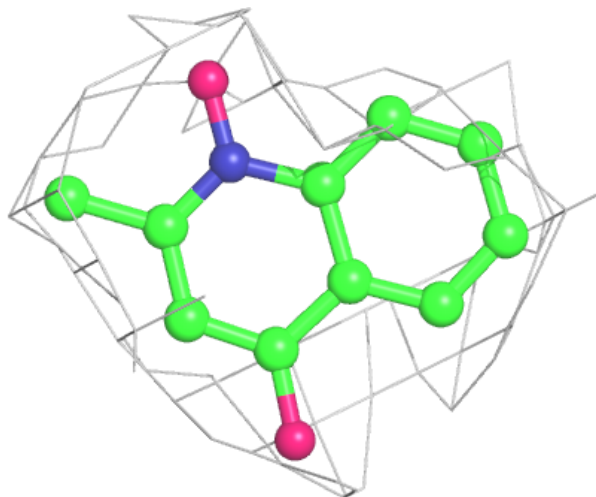
Electron density around HQO E 1004:

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



Electron density around HQO A 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 ⓘ

There are no such residues in this entry.