



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 04:16 PM JST

PDB ID : 6KOE / pdb_00006koe
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 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 : 1.8.5 (274361), CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

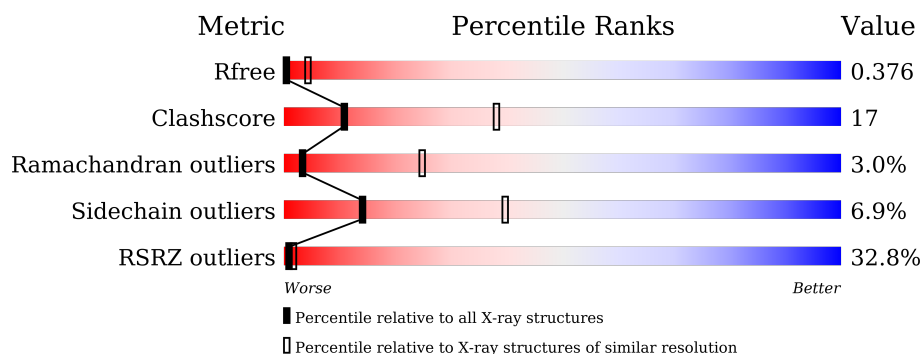
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.75 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}	180053	1029 (3.90-3.62)
Clashscore	190562	1061 (3.90-3.62)
Ramachandran outliers	187476	1014 (3.90-3.62)
Sidechain outliers	187428	1009 (3.90-3.62)
RSRZ outliers	180081	1028 (3.90-3.62)

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	655	
1	E	655	
2	B	296	
2	F	296	
3	C	204	
3	G	204	

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Mol	Chain	Length	Quality of chain
4	D	124	17%39%16%•44%
4	H	124	12%40%16%•44%

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			

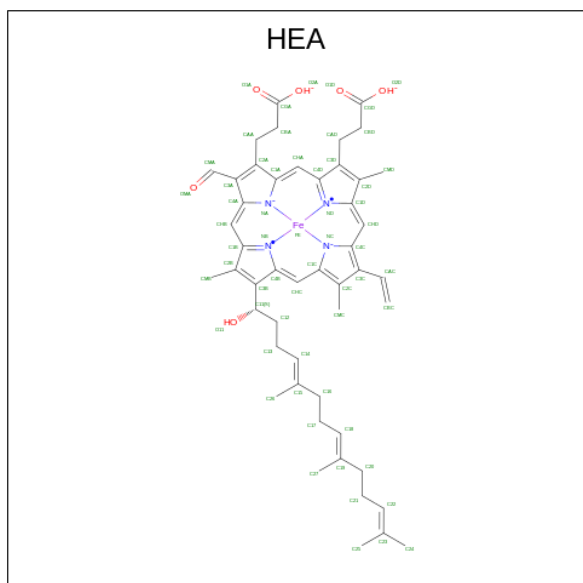
- Molecule 3 is a protein called AA3-600 quinol oxidase subunit IIII.

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 (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).

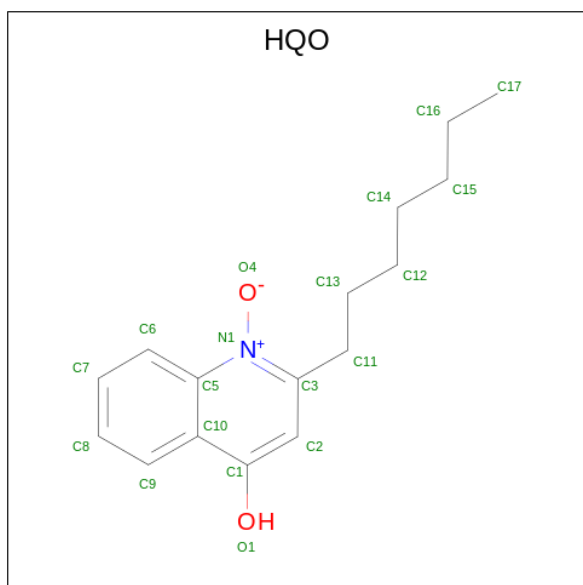


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
5	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
5	E	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
5	E	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 6 is COPPER (II) ION (CCD ID: 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 (CCD ID: HQO) (formula: $C_{16}H_{21}NO_2$).



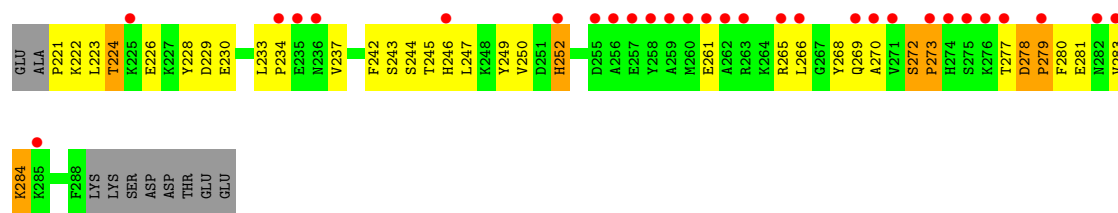
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 13 10 1 2	0	0
7	E	1	Total C N O 13 10 1 2	0	0

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.

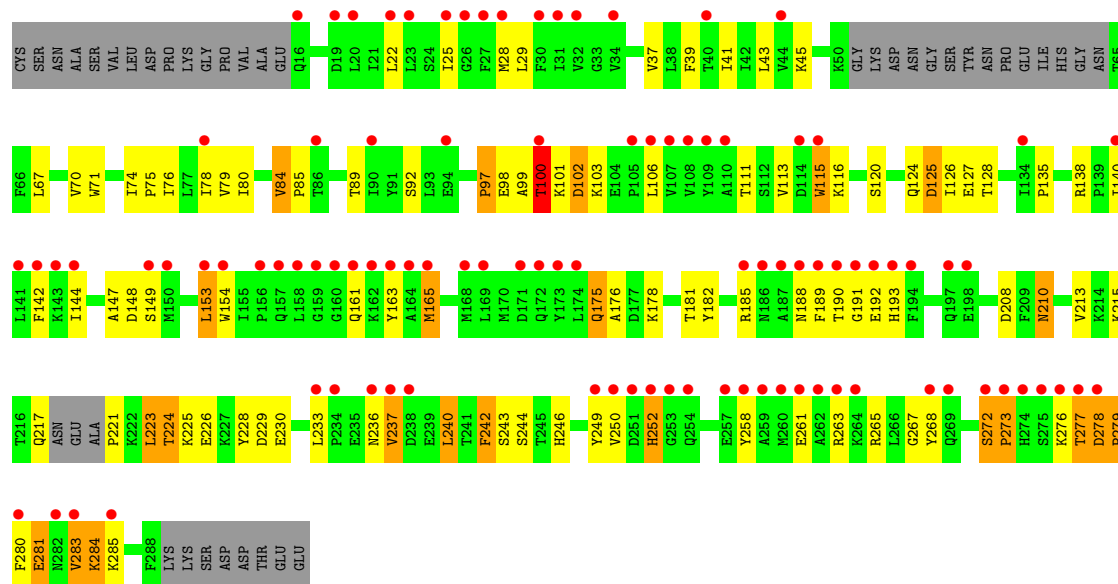
- [illegible]

- Molecule 1: AA3-600 quinol oxidase subunit I

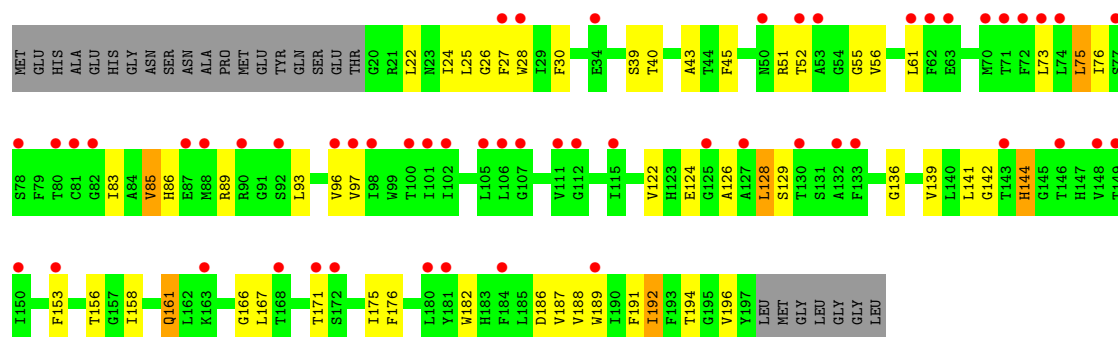




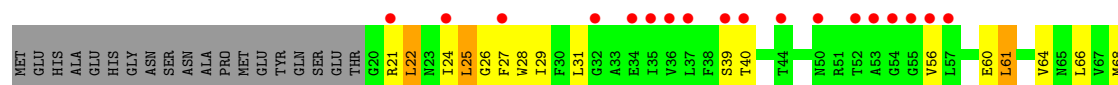
• Molecule 2: Quinol oxidase subunit 2

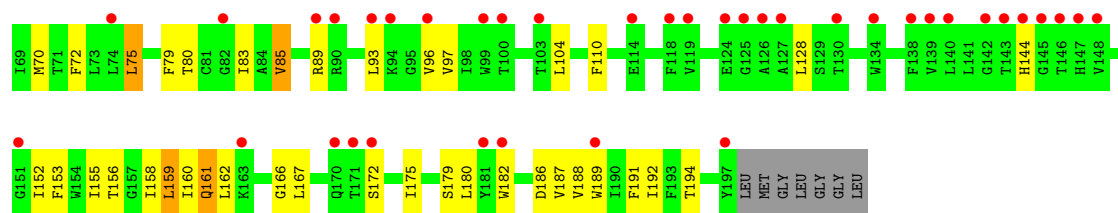


• Molecule 3: AA3-600 quinol oxidase subunit IIII

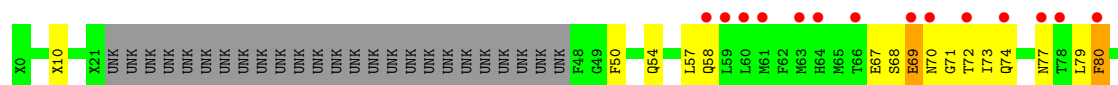
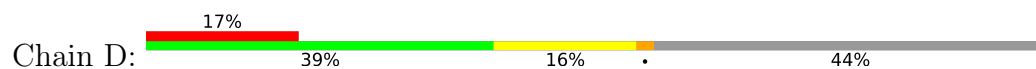


• Molecule 3: AA3-600 quinol oxidase subunit IIII

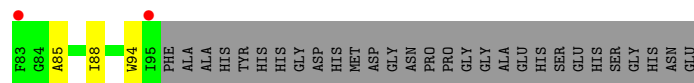
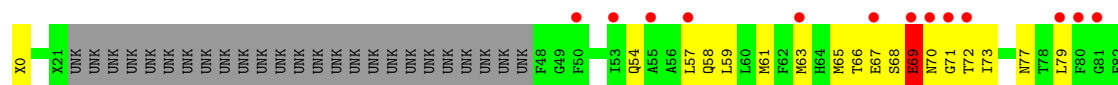




● Molecule 4: AA3-600 quinol oxidase subunit IV



● Molecule 4: AA3-600 quinol oxidase subunit IV



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 0.350 , 0.376	Depositor DCC
R_{free} test set	1996 reflections (3.82%)	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)	0.20 , 17.8	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	0.79	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: CU, HQO, 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	0.17	0/5022	0.39	0/6827
1	E	0.17	0/5022	0.39	0/6827
2	B	0.18	0/2122	0.43	0/2879
2	F	0.20	0/2122	0.46	0/2879
3	C	0.18	0/1452	0.40	0/1974
3	G	0.16	0/1452	0.36	0/1974
4	D	0.18	0/381	0.36	0/514
4	H	0.14	0/381	0.33	0/514
All	All	0.17	0/17954	0.40	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	188	0
1	E	4855	0	4855	180	0
2	B	2073	0	2061	85	0
2	F	2073	0	2061	73	0
3	C	1411	0	1444	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1411	0	1444	46	0
4	D	482	0	395	16	0
4	H	482	0	395	23	0
5	A	120	0	106	16	0
5	E	120	0	106	10	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	592	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 17.

All (592) 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:349:MET:HE1	1:A:395:VAL:HG23	1.60	0.81
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:E:349:MET:HE1	1:E:395:VAL:HG23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:607:TRP:CD1	1:E:612:VAL:H	2.07	0.72
1:A:54:LYS:NZ	1:A:545:PRO:O	2.21	0.72
2:F:102:ASP:OD2	2:F:102:ASP:N	2.21	0.71
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:298:ILE:HD12	1:E:377:MET:HE1	1.75	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
2:F:37:VAL:HG13	2:F:41:ILE:HD12	1.76	0.68
1:E:470:LEU:HD11	1:E:492:ASN:HA	1.74	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:20:GLN:O	1:A:24:ALA:N	2.25	0.66
1:A:94:HIS:NE2	7:A:1004:HQO:O1	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:175:GLN:NE2	2:F:176:ALA:O	2.30	0.65
2:F:178:LYS:O	2:F:182:TYR:OH	2.13	0.64
1:E:286:VAL:O	1:E:424:THR:OG1	2.14	0.64
1:A:53:HIS:CD2	1:A:131:ASP:HA	2.33	0.64
1:A:97:GLU:HB2	7:A:1004:HQO:HC8	1.79	0.64
3:C:22:LEU:HD23	3:C:22:LEU:H	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:B:233:LEU:HD13	2:B:284:LYS:HZ3	1.63	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: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:123:VAL:HG13	1:E:225:THR:HG23	1.82	0.62
1:E:420:LEU:HD13	5:E:1002:HEA:HBC2	1.82	0.62
1:E:414:SER:OG	1:E:464:PHE:O	2.18	0.61
1:A:425:VAL:HG21	5:A:1001:HEA:HMC3	1.83	0.61
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
1:E:371:ILE:HD11	1:E:377:MET:HE2	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
3:G:79:PHE:HE2	3:G:179:SER:HA	1.66	0.60
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
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:E:133:ALA:HA	1:E:211:MET:HE1	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:LYS:HZ1	1:E:544:PRO:HB2	1.67	0.59
2:F:228:TYR:HD2	2:F:249:TYR:HD2	1.48	0.59
1:E:445:ASN:HB3	1:E:448:ILE:HD11	1.82	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
2:F:165:MET:HE1	1:E:269:MET:HB3	1.84	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:92:SER:O	1:A:96:ASN:ND2	2.36	0.58
1:A:212:ARG:HH12	1:A:218:LEU:HD12	1.68	0.58
1:E:96:ASN:N	1:E:96:ASN:HD22	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:54:LYS:NZ	1:E:544:PRO:HB2	2.19	0.58
1:E:426:PHE:O	1:E:430:ALA:N	2.30	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
3:G:156:THR:HA	3:G:159:LEU:HB2	1.86	0.58
1:A:116:ILE:HG13	1:A:232:MET:HE1	1.85	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
2:F:230:GLU:O	2:F:284:LYS:NZ	2.38	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:B:109:TYR:HA	2:B:143:LYS:HB2	1.86	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
1:E:337:SER:O	1:E:339:SER:N	2.36	0.57
3:C:141:LEU:HA	3:C:144:HIS:HB3	1.85	0.57
2:B:269:GLN:NE2	2:F:281:GLU:OE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:272:SER:OG	2:F:273:PRO:HD3	2.04	0.57
2:F:190:THR:HB	1:E:478:ARG:HB3	1.86	0.56
1:E:174:SER:HA	1:E:253:ARG:HH11	1.69	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
3:G:175:ILE:O	3:G:179:SER:OG	2.21	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
3:C:93:LEU:HD23	3:C:93:LEU:H	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
3:G:93:LEU:HD23	3:G:93:LEU:H	1.71	0.55
1:E:115:LEU:HG	1:E:289:PRO:HB2	1.88	0.55
3:C:73:LEU:HD12	3:C:76:ILE:HD11	1.87	0.55
3:C:153:PHE:HA	3:C:156:THR:HG22	1.88	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:79:ARG:NH2	1:A:467:GLN:OE1	2.35	0.55
1:A:107:ILE:HA	1:A:111:ALA:HB3	1.88	0.55
1:A:367:TYR:C	1:A:369:GLY:H	2.13	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:274:LEU:HD22	3:C:40:THR:HG23	1.89	0.55
2:B:223:LEU:N	2:B:244:SER:HB3	2.21	0.55
1:E:54:LYS:NZ	1:E:548:ASN:HB3	2.22	0.55
1:A:607:TRP:CD1	1:A:612:VAL:H	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:THR:HG21	2:B:252:HIS:CD2	2.42	0.54
3:G:194:THR:HG21	4:H:54:GLN:HG3	1.89	0.54
1:E:48:ILE:HA	1:E:143:TRP:HZ2	1.72	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
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
2:F:185:ARG:HD3	1:E:476:PRO:HG2	1.88	0.54
1:E:437:PRO:HG3	1:E:443:LYS:HB3	1.89	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
3:G:162:LEU:HD23	3:G:166:GLY:HA2	1.90	0.53
2:F:190:THR:OG1	1:E:96:ASN:OD1	2.15	0.53
2:F:272:SER:HB3	1:E:179:PRO:HB3	1.91	0.53
2:B:250:VAL:C	2:B:252:HIS:H	2.17	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:47:TRP:O	1:A:49:THR:N	2.42	0.52
1:A:376:PRO:HB3	1:A:434:PHE:HB2	1.90	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:57:GLY:HA3	1:A:121:VAL:HG23	1.91	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
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:298:ILE:HD12	1:A:377:MET:HE1	1.92	0.52
1:A:106:MET:HA	1:A:110:MET:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:VAL:HG13	1:E:438:LYS:HZ3	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
2:F:276:LYS:HD2	2:F:278:ASP:H	1.74	0.52
1:E:96:ASN:HD22	1:E:96:ASN:H	1.56	0.52
1:E:294:PHE:HZ	1:E:426:PHE:HB3	1.75	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:96:ASN:OD1	2:B:190:THR:OG1	2.22	0.51
1:A:107:ILE:O	1:A:112:MET:HB2	2.10	0.51
1:A:277:ILE:HD13	4:D:88:ILE:HG12	1.93	0.51
1:A:304:LYS:HG2	1:A:305:GLN:H	1.74	0.51
2:B:157:GLN:HG3	2:B:182:TYR:HA	1.91	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
2:F:250:VAL:C	2:F:252:HIS:H	2.19	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: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: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
2:B:127:GLU:CD	2:B:246:HIS:HD2	2.20	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:E:240:PRO:O	1:E:244:VAL:HG22	2.12	0.50
1:A:506:PHE:CG	5:A:1001:HEA:H162	2.46	0.50
3:G:167:LEU:HB3	3:G:172:SER:HB2	1.94	0.50
2:F:154:TRP:HA	2:F:161:GLN:HB3	1.94	0.50
1:E:223:MET:HE3	1:E:312:MET:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:588:ARG:NE	1:E:624:LEU:HB3	2.26	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:56:LEU:HD21	1:A:139:ASN:HA	1.94	0.50
1:A:301:PHE:HB2	1:A:377:MET:SD	2.52	0.50
2:F:217:GLN:OE1	2:F:217:GLN:N	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
4:H:94:TRP:NE1	1:E:340:VAL:HG12	2.26	0.49
1:E:156:PHE:HE1	7:E:1004:HQO:C5	2.24	0.49
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:H	1:A:96:ASN:HD22	1.61	0.49
1:E:141:SER:OG	1:E:200:THR:OG1	2.26	0.49
3:G:28:TRP:HZ2	4:H:66:THR:HG22	1.78	0.49
2:F:89:THR:HA	2:F:92:SER:HB3	1.94	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
3:G:22:LEU:O	3:G:26:GLY:N	2.28	0.48
1:E:607:TRP:HD1	1:E:612:VAL:H	1.56	0.48
2:F:101:LYS:HE3	2:F:102:ASP:OD2	2.13	0.48
1:E:177:MET:HG2	1:E:179:PRO:HD2	1.94	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
2:F:223:LEU:HD22	2:F:225:LYS:H	1.78	0.48
1:E:606:GLU:HB3	1:E:607:TRP:CE3	2.48	0.48
1:A:191:GLN:OE1	1:A:246:LEU:HB2	2.14	0.48
2:F:100:THR:OG1	2:F:101:LYS:N	2.45	0.48
1:E:280:HIS:HA	1:E:283:VAL:HB	1.95	0.48
1:A:95:TYR:HA	1:A:98:ILE:HB	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:G:39:SER:HB2	4:H:85:ALA:HA	1.95	0.48
2:F:223:LEU:N	2:F:244:SER:HB3	2.29	0.48
3:G:75:LEU:HD11	3:G:182:TRP:NE1	2.29	0.47
2:F:135:PRO:HG2	2:F:138:ARG:HD2	1.96	0.47
1:E:460:PHE:HA	1:E:502:MET:SD	2.53	0.47
1:E:539:THR:OG1	1:E:541:SER:O	2.31	0.47
1:A:116:ILE:O	1:A:120:ASN:N	2.34	0.47
1:A:509:LEU:O	1:A:513:ILE:HG13	2.15	0.47
3:G:161:GLN:OE1	3:G:162:LEU:HG	2.13	0.47
2:F:67:LEU:O	2:F:70:VAL:HG12	2.13	0.47
1:E:212:ARG:HH12	1:E:218:LEU:HD12	1.79	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:96:ASN:HD22	1:A:96:ASN:N	2.13	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
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:63:SER:O	1:A:67:MET:HG2	2.14	0.47
1:A:218:LEU:HA	1:A:221:MET:HE3	1.97	0.47
1:E:32:PHE:HA	1:E:36:TYR:HB2	1.96	0.47
1:A:68:LEU:HD22	5:A:1001:HEA:H262	1.97	0.47
1:A:136:TYR:OH	1:A:588:ARG:HD3	2.14	0.47
1:A:353:ILE:HB	1:A:354:PRO:HD3	1.96	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
3:C:86:HIS:HE1	3:C:96:VAL:HA	1.80	0.47
2:F:43:LEU:O	2:F:45:LYS:N	2.44	0.47
1:E:166:TRP:H	5:E:1001:HEA:CGD	2.28	0.47
1:A:68:LEU:O	1:A:72:GLY:N	2.48	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
3:C:187:VAL:HG13	4:D:58:GLN:HG3	1.97	0.47
2:F:190:THR:HG21	1:E:99:PHE:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:PHE:H	1:E:240:PRO:CD	2.28	0.47
1:E:607:TRP:CD1	1:E:611:GLY:HA2	2.49	0.47
1:A:349:MET:HE3	1:A:398:ALA:HB3	1.96	0.47
3:G:85:VAL:HA	3:G:89:ARG:HB2	1.97	0.47
1:E:204:PHE:HB2	1:E:232:MET:HG3	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:92:SER:O	1:E:96:ASN:ND2	2.49	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:A:206:VAL:HG21	3:C:26:GLY:HA2	1.97	0.46
2:B:80:ILE:HA	2:B:83:SER:HB3	1.98	0.46
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
3:G:187:VAL:HG13	4:H:58:GLN:HB3	1.97	0.46
1:E:444:LEU:HG	1:E:512:ASN:HB3	1.96	0.46
1:A:223:MET:HE3	1:A:312:MET:HG2	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
2:F:101:LYS:HE2	2:F:103:LYS:HG2	1.96	0.46
1:E:282:GLU:HA	1:E:285:ILE:HD12	1.96	0.46
2:F:240:LEU:HD12	2:F:242:PHE:HE1	1.80	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
3:G:188:VAL:HA	3:G:191:PHE:HB2	1.98	0.46
1:E:416:PHE:CE2	5:E:1001:HEA:HHD	2.50	0.46
1:A:96:ASN:HA	1:A:99:PHE:HD1	1.80	0.46
1:A:396:MET:O	1:A:406:TYR:OH	2.29	0.46
2:B:191:GLY:O	2:B:193:HIS:N	2.49	0.46
3:G:21:ARG:HA	3:G:21:ARG:HD3	1.66	0.46
1:E:283:VAL:HG13	5:E:1002:HEA:C3C	2.46	0.46
2:B:80:ILE:HD12	2:B:83:SER:HB3	1.96	0.46
2:B:114:ASP:O	2:B:116:LYS:N	2.47	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:45:SER:O	1:E:585:ASN:ND2	2.49	0.45
1:E:367:TYR:C	1:E:369:GLY:H	2.23	0.45
1:E:432:PHE:HB3	1:E:433:ILE:HD12	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:213:THR:OG1	1:A:552:LEU:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:PHE:O	1:A:430:ALA:N	2.40	0.45
3:C:55:GLY:C	2:F:225:LYS:HE3	2.41	0.45
3:C:188:VAL:HG23	3:C:189:TRP:HE3	1.80	0.45
1:E:349:MET:HE3	1:E:398:ALA:HB3	1.96	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
2:B:114:ASP:C	2:B:116:LYS:H	2.24	0.45
2:F:250:VAL:HG21	2:F:258:TYR:CD1	2.52	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:B:112:SER:O	2:B:146:SER:OG	2.34	0.45
2:B:125:ASP:C	2:B:126:ILE:HG13	2.42	0.45
2:F:120:SER:HA	2:F:127:GLU:HA	1.99	0.45
1:E:418:TYR:HA	1:E:460:PHE:HZ	1.81	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:96:ASN:HA	1:E:99:PHE:CD1	2.51	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:A:24:ALA:O	1:A:28:ILE:HG12	2.17	0.45
1:A:154:ILE:C	1:A:156:PHE:H	2.24	0.45
1:A:210:LYS:NZ	4:D:70:ASN:OD1	2.49	0.45
1:A:344:PHE:O	1:A:348:THR:OG1	2.21	0.45
3:C:73:LEU:HD23	4:D:10:UNK:HA	1.99	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
2:F:228:TYR:HD2	2:F:249:TYR:CD2	2.33	0.45
1:E:178:SER:OG	1:E:179:PRO:HD3	2.17	0.45
1:A:60:TYR:HB3	1:A:113:PRO:O	2.17	0.44
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
2:B:224:THR:O	2:B:224:THR:OG1	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:179:PRO:HG3	2:B:272:SER:HB3	1.98	0.44
1:A:283:VAL:HG13	5:A:1002:HEA:C3C	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:LEU:HD23	5:A:1001:HEA:HAC	1.99	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:37:VAL:HG13	2:B:41:ILE:HD12	1.98	0.44
2:B:117:TRP:HB3	2:B:119:PHE:CE2	2.53	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
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
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
3:G:96:VAL:HB	3:G:162:LEU:CD1	2.48	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
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
1:A:140:LEU:O	1:A:144:THR:OG1	2.25	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
2:F:115:TRP:CZ2	2:F:236:ASN:HA	2.53	0.43
1:E:96:ASN:HA	1:E:99:PHE:HD1	1.84	0.43
1:E:376:PRO:HB3	1:E:434:PHE:HB2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:H:67:GLU:HA	4:H:68:SER:HA	1.73	0.43
2:F:111:THR:HG21	2:F:252:HIS:CD2	2.54	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
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
1:A:257:ALA:HB2	3:C:128:LEU:HD13	2.00	0.42
1:A:588:ARG:NE	1:A:624:LEU:HB3	2.34	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
4:H:57:LEU:HD22	4:H:58:GLN:HE22	1.84	0.42
1:E:238:ALA:HB2	1:E:324:PHE:CE2	2.54	0.42
1:E:304:LYS:HG2	1:E:305:GLN:H	1.83	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
3:G:29:ILE:HA	4:H:77:ASN:OD1	2.18	0.42
1:E:416:PHE:HZ	5:E:1001:HEA:HHD	1.82	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
2:F:233:LEU:HD13	2:F:284:LYS:HZ3	1.83	0.42
1:E:412:LEU:HD11	5:E:1002:HEA:HHA	2.01	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:110:MET:C	1:A:113:PRO:HD2	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:G:26:GLY:HA3	1:E:134:PHE:CZ	2.55	0.42
1:E:144:THR:O	1:E:192:ILE:HG22	2.20	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
3:G:80:THR:HG23	4:H:65:MET:HE1	2.02	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:E:195:ILE:HD13	1:E:195:ILE:HA	1.91	0.41
1:E:344:PHE:O	1:E:348:THR:OG1	2.27	0.41
3:G:66:LEU:O	3:G:70:MET:HB2	2.20	0.41
3:G:155:ILE:O	3:G:159:LEU:HD23	2.20	0.41
2:F:191:GLY:O	2:F:193:HIS:N	2.53	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: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
3:G:61:LEU:HD12	3:G:64:VAL:HG23	2.03	0.41
1:E:97:GLU:HA	1:E:162:PRO:O	2.20	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:A:115:LEU:HD12	1:A:115:LEU:HA	1.80	0.41
1:A:310:LYS:HE2	2:B:65:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ALA:HB3	1:A:354:PRO:HB3	2.03	0.41
3:C:141:LEU:CA	3:C:144:HIS:HB3	2.50	0.41
3:G:79:PHE:CE2	3:G:179:SER:HA	2.50	0.41
3:G:161:GLN:CD	3:G:162:LEU:HG	2.46	0.41
3:G:180:LEU:HD11	4:H:65:MET:HB2	2.01	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
1:E:170:MET:N	1:E:171:PRO:HD2	2.36	0.41
1:E:298:ILE:HG21	1:E:362:TRP:CD1	2.56	0.41
1:A:305:GLN:O	1:A:365:THR:HG23	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
2:F:149:SER:HB3	1:E:176:ASP:OD2	2.21	0.41
1:E:313:VAL:O	1:E:316:ILE:HG22	2.21	0.41
1:A:79:ARG:NH2	1:A:495:SER:HB3	2.28	0.40
1:A:170:MET:N	1:A:171:PRO:HD2	2.36	0.40
1:A:334:MET:HB3	2:B:163:TYR:CD2	2.56	0.40
1:A:506:PHE:CD1	5:A:1001:HEA:H261	2.55	0.40
3:C:139:VAL:C	3:C:142:GLY:H	2.29	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
2:F:163:TYR:HB2	1:E:334:MET:HA	2.04	0.40
1:E:190:LEU:HB2	1:E:246:LEU:HD11	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
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:74:ILE:O	2:F:78:ILE:HG12	2.21	0.40
2:F:228:TYR:CD2	2:F:249:TYR:HD2	2.34	0.40
1:E:82:LEU:HD11	1:E:95:TYR:OH	2.20	0.40
2:F:106:LEU:HD23	2:F:140:ILE:HG22	2.04	0.40
2:B:278:ASP:O	2:B:279:PRO:C	2.64	0.40
2:F:80:ILE:HD12	2:F:80:ILE:HA	1.95	0.40
1:E:306:LEU:HD23	1:E:365:THR:HG21	2.03	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	603/655 (92%)	509 (84%)	76 (13%)	18 (3%)	3	25
1	E	603/655 (92%)	510 (85%)	77 (13%)	16 (3%)	4	26
2	B	250/296 (84%)	188 (75%)	49 (20%)	13 (5%)	1	16
2	F	250/296 (84%)	189 (76%)	48 (19%)	13 (5%)	1	16
3	C	176/204 (86%)	154 (88%)	21 (12%)	1 (1%)	21	52
3	G	176/204 (86%)	157 (89%)	19 (11%)	0	100	100
4	D	46/124 (37%)	37 (80%)	7 (15%)	2 (4%)	2	19
4	H	46/124 (37%)	37 (80%)	7 (15%)	2 (4%)	2	19
All	All	2150/2558 (84%)	1781 (83%)	304 (14%)	65 (3%)	3	25

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	486 (95%)	26 (5%)	21	45
1	E	512/558 (92%)	482 (94%)	30 (6%)	18	43
2	B	230/263 (88%)	213 (93%)	17 (7%)	13	38
2	F	230/263 (88%)	203 (88%)	27 (12%)	5	22
3	C	151/171 (88%)	141 (93%)	10 (7%)	15	41
3	G	151/171 (88%)	137 (91%)	14 (9%)	8	31
4	D	38/59 (64%)	35 (92%)	3 (8%)	11	36
4	H	38/59 (64%)	36 (95%)	2 (5%)	20	45
All	All	1862/2102 (89%)	1733 (93%)	129 (7%)	14	40

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ARG
1	A	93	ASN
1	A	96	ASN
1	A	97	GLU
1	A	105	ILE
1	A	114	PHE
1	A	115	LEU
1	A	120	ASN
1	A	145	PHE

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Mol	Chain	Res	Type
1	A	151	LEU
1	A	172	LEU
1	A	187	LEU
1	A	208	ILE
1	A	216	MET
1	A	251	PHE
1	A	260	PHE
1	A	273	ASN
1	A	283	VAL
1	A	288	LEU
1	A	349	MET
1	A	363	LEU
1	A	395	VAL
1	A	416	PHE
1	A	500	PHE
1	A	552	LEU
1	A	581	HIS
2	B	20	LEU
2	B	29	LEU
2	B	39	PHE
2	B	103	LYS
2	B	115	TRP
2	B	128	THR
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	237	VAL
2	B	252	HIS
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

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Mol	Chain	Res	Type
3	C	161	GLN
3	C	192	ILE
4	D	69	GLU
4	D	79	LEU
4	D	80	PHE
3	G	22	LEU
3	G	25	LEU
3	G	56	VAL
3	G	60	GLU
3	G	61	LEU
3	G	75	LEU
3	G	83	ILE
3	G	85	VAL
3	G	97	VAL
3	G	128	LEU
3	G	159	LEU
3	G	160	ILE
3	G	161	GLN
3	G	192	ILE
4	H	69	GLU
4	H	79	LEU
2	F	22	LEU
2	F	25	ILE
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	128	THR
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	210	ASN
2	F	213	VAL
2	F	215	LYS
2	F	223	LEU
2	F	224	THR
2	F	237	VAL

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Mol	Chain	Res	Type
2	F	246	HIS
2	F	252	HIS
2	F	272	SER
2	F	277	THR
2	F	283	VAL
2	F	284	LYS
1	E	79	ARG
1	E	93	ASN
1	E	96	ASN
1	E	97	GLU
1	E	104	THR
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	187	LEU
1	E	208	ILE
1	E	216	MET
1	E	239	PHE
1	E	260	PHE
1	E	273	ASN
1	E	283	VAL
1	E	316	ILE
1	E	340	VAL
1	E	349	MET
1	E	351	ILE
1	E	363	LEU
1	E	395	VAL
1	E	415	HIS
1	E	416	PHE
1	E	500	PHE
1	E	552	LEU
1	E	565	LYS
1	E	581	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	139	ASN

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Mol	Chain	Res	Type
1	A	184	ASN
1	A	329	HIS
1	A	473	GLN
2	B	175	GLN
2	B	246	HIS
2	B	252	HIS
4	H	58	GLN
2	F	188	ASN
2	F	210	ASN
1	E	184	ASN
1	E	415	HIS

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	$\# Z > 2$
7	HQO	A	1004	1	14,14,20	3.23	3 (21%)	13,20,26	1.43	1 (7%)
7	HQO	E	1004	-	14,14,20	3.20	3 (21%)	13,20,26	1.49	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	HEA	E	1002	1	66,67,67	2.50	25 (37%)	78,103,103	2.74	34 (43%)
5	HEA	A	1001	1	66,67,67	2.59	27 (40%)	78,103,103	2.50	32 (41%)
5	HEA	E	1001	1	66,67,67	2.62	27 (40%)	78,103,103	2.48	29 (37%)
5	HEA	A	1002	1	66,67,67	2.48	26 (39%)	78,103,103	2.81	36 (46%)

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
7	HQO	A	1004	1	-	-	0/2/2/2
7	HQO	E	1004	-	-	-	0/2/2/2
5	HEA	E	1002	1	-	8/36/76/76	-
5	HEA	A	1001	1	-	9/36/76/76	-
5	HEA	E	1001	1	-	9/36/76/76	-
5	HEA	A	1002	1	-	7/36/76/76	-

All (111) 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	5.95	1.49	1.36
5	E	1002	HEA	FE-NB	5.84	2.13	1.94
5	E	1001	HEA	C3B-C2B	5.82	1.47	1.34
5	A	1001	HEA	C3B-C2B	5.72	1.47	1.34
5	A	1001	HEA	C3A-C2A	5.71	1.49	1.36
5	A	1002	HEA	FE-NB	5.70	2.12	1.94
5	E	1002	HEA	C3B-C2B	5.65	1.47	1.34
5	E	1002	HEA	FE-ND	5.55	2.12	1.94
5	A	1002	HEA	C3B-C2B	5.53	1.47	1.34
5	A	1002	HEA	FE-ND	5.50	2.11	1.94
5	A	1001	HEA	C3D-C2D	5.33	1.48	1.36
5	E	1002	HEA	C3A-C2A	5.31	1.48	1.36
5	E	1001	HEA	FE-ND	5.29	2.11	1.94
5	E	1001	HEA	C3D-C2D	5.27	1.47	1.36
5	A	1001	HEA	FE-NB	5.15	2.10	1.94
5	A	1002	HEA	C3A-C2A	5.12	1.47	1.36
5	E	1002	HEA	C3D-C2D	5.07	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	HEA	FE-ND	5.07	2.10	1.94
5	E	1001	HEA	FE-NB	5.03	2.10	1.94
5	A	1001	HEA	CHB-C4A	5.02	1.48	1.38
5	A	1002	HEA	C3D-C2D	4.94	1.47	1.36
5	E	1001	HEA	CHB-C4A	4.90	1.47	1.38
5	A	1001	HEA	CHD-C1D	4.87	1.48	1.38
5	A	1002	HEA	FE-NC	4.87	2.11	1.95
5	E	1002	HEA	FE-NC	4.83	2.11	1.95
5	E	1001	HEA	CHA-C1A	4.80	1.47	1.38
5	E	1001	HEA	FE-NC	4.71	2.11	1.95
5	E	1001	HEA	CHD-C1D	4.69	1.48	1.38
5	A	1001	HEA	CHA-C1A	4.68	1.47	1.38
5	A	1001	HEA	CHC-C4B	4.62	1.47	1.38
5	E	1001	HEA	CHC-C4B	4.57	1.47	1.38
5	A	1001	HEA	FE-NC	4.54	2.10	1.95
5	E	1002	HEA	CHD-C1D	4.45	1.47	1.38
5	A	1002	HEA	CHB-C4A	4.44	1.47	1.38
5	A	1002	HEA	CHC-C4B	4.43	1.47	1.38
5	E	1002	HEA	CHB-C4A	4.36	1.46	1.38
5	A	1002	HEA	CHD-C1D	4.29	1.47	1.38
5	E	1002	HEA	CHA-C1A	4.24	1.46	1.38
5	E	1002	HEA	CHC-C4B	4.20	1.47	1.38
5	A	1002	HEA	CHA-C1A	4.18	1.46	1.38
5	A	1002	HEA	C1A-NA	3.99	1.47	1.39
5	E	1001	HEA	C1A-NA	3.96	1.47	1.39
5	A	1001	HEA	CHB-C1B	3.92	1.48	1.39
5	A	1001	HEA	CHD-C4C	3.90	1.48	1.39
5	A	1001	HEA	C1A-NA	3.88	1.47	1.39
5	E	1001	HEA	CHB-C1B	3.88	1.48	1.39
5	E	1001	HEA	C4A-NA	3.86	1.47	1.39
5	E	1002	HEA	C1A-NA	3.78	1.47	1.39
5	A	1001	HEA	CHC-C1C	3.74	1.47	1.39
5	E	1001	HEA	CHD-C4C	3.69	1.47	1.39
5	E	1001	HEA	CHC-C1C	3.63	1.47	1.39
5	A	1001	HEA	CHA-C4D	3.62	1.47	1.39
5	A	1001	HEA	C4A-NA	3.62	1.46	1.39
5	A	1002	HEA	C4A-NA	3.62	1.46	1.39
5	E	1002	HEA	CHD-C4C	3.61	1.47	1.39
5	E	1002	HEA	C4A-NA	3.60	1.46	1.39
5	A	1002	HEA	CHC-C1C	3.60	1.47	1.39
5	E	1001	HEA	CHA-C4D	3.54	1.47	1.39
7	E	1004	HQO	C10-C5	3.50	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1004	HQO	C10-C5	3.46	1.48	1.42
5	A	1002	HEA	CHD-C4C	3.45	1.47	1.39
5	E	1002	HEA	CHC-C1C	3.43	1.47	1.39
5	A	1002	HEA	CHB-C1B	3.42	1.47	1.39
5	E	1002	HEA	CHB-C1B	3.28	1.46	1.39
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	E	1002	HEA	CHA-C4D	3.19	1.46	1.39
5	A	1002	HEA	CHA-C4D	3.10	1.46	1.39
5	E	1001	HEA	C1A-C2A	3.10	1.50	1.45
5	A	1002	HEA	C4B-C3B	2.92	1.49	1.44
5	A	1001	HEA	C1A-C2A	2.89	1.50	1.45
5	A	1001	HEA	C1D-ND	-2.88	1.35	1.40
5	E	1001	HEA	C4B-C3B	2.84	1.49	1.44
5	E	1001	HEA	C1D-ND	-2.84	1.35	1.40
5	A	1001	HEA	C4B-C3B	2.83	1.49	1.44
5	E	1002	HEA	C4B-C3B	2.82	1.49	1.44
5	A	1001	HEA	C4B-NB	-2.80	1.35	1.40
5	E	1001	HEA	C4B-NB	-2.69	1.35	1.40
5	E	1001	HEA	C1C-C2C	2.68	1.49	1.43
5	E	1002	HEA	C3C-C4C	2.67	1.49	1.42
5	A	1001	HEA	C3C-C4C	2.65	1.49	1.42
5	A	1002	HEA	C1D-ND	-2.62	1.35	1.40
5	E	1001	HEA	C4D-C3D	2.61	1.49	1.45
5	E	1001	HEA	C3C-C4C	2.57	1.48	1.42
5	E	1002	HEA	C1B-C2B	2.56	1.49	1.44
5	E	1002	HEA	C4B-NB	-2.55	1.35	1.40
5	E	1002	HEA	C1D-ND	-2.55	1.35	1.40
5	A	1001	HEA	C1C-C2C	2.48	1.49	1.43
5	A	1002	HEA	C1A-C2A	2.48	1.49	1.45
5	A	1002	HEA	C1C-C2C	2.45	1.49	1.43
5	A	1001	HEA	C1B-C2B	2.45	1.49	1.44
5	E	1001	HEA	C1D-C2D	2.43	1.49	1.44
5	A	1002	HEA	C4B-NB	-2.43	1.36	1.40
5	A	1002	HEA	C3C-C4C	2.41	1.48	1.42
5	E	1001	HEA	CMA-C3A	2.40	1.50	1.45
5	E	1002	HEA	C1D-C2D	2.40	1.49	1.44
5	A	1002	HEA	C1B-C2B	2.38	1.49	1.44
5	E	1002	HEA	C1C-C2C	2.37	1.48	1.43
5	A	1001	HEA	C1D-C2D	2.37	1.49	1.44
5	E	1002	HEA	C1A-C2A	2.36	1.49	1.45
5	A	1002	HEA	C1D-C2D	2.31	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1002	HEA	C4D-C3D	2.28	1.49	1.45
5	A	1001	HEA	C4C-NC	-2.27	1.35	1.39
5	E	1001	HEA	C4C-NC	-2.27	1.35	1.39
5	E	1001	HEA	C1B-C2B	2.23	1.48	1.44
5	A	1001	HEA	C4D-C3D	2.23	1.48	1.45
5	A	1001	HEA	C1C-NC	-2.09	1.35	1.39
5	A	1002	HEA	C4D-C3D	2.08	1.48	1.45
5	A	1002	HEA	C4C-NC	-2.01	1.35	1.39

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1002	HEA	C3C-C4C-NC	7.28	114.72	110.25
5	E	1002	HEA	C3D-C4D-ND	7.11	117.24	110.36
5	A	1002	HEA	C3D-C4D-ND	6.85	116.99	110.36
5	E	1002	HEA	C3C-C4C-NC	6.61	114.31	110.25
5	E	1001	HEA	C3C-C4C-NC	6.19	114.06	110.25
5	E	1002	HEA	C2B-C1B-NB	6.18	117.28	109.88
5	E	1001	HEA	CHA-C1A-NA	-6.01	117.94	124.44
5	A	1002	HEA	C2B-C1B-NB	6.00	117.07	109.88
5	A	1001	HEA	CHA-C1A-NA	-5.99	117.96	124.44
5	E	1001	HEA	C3D-C4D-ND	5.85	116.03	110.36
5	E	1001	HEA	CHA-C4D-ND	-5.85	118.06	124.42
5	E	1002	HEA	C3B-C4B-NB	5.79	116.70	109.84
5	E	1001	HEA	C3C-C2C-C1C	-5.67	100.32	107.16
5	A	1001	HEA	C3C-C4C-NC	5.66	113.73	110.25
5	A	1002	HEA	C2A-C1A-NA	5.63	115.80	110.32
5	E	1002	HEA	C3C-C2C-C1C	-5.61	100.39	107.16
5	A	1001	HEA	C3D-C4D-ND	5.49	115.67	110.36
5	A	1002	HEA	C3C-C2C-C1C	-5.45	100.58	107.16
5	E	1002	HEA	C2A-C1A-NA	5.31	115.49	110.32
5	A	1002	HEA	C2D-C1D-ND	5.29	116.11	109.84
5	A	1002	HEA	C3B-C4B-NB	5.22	116.02	109.84
5	A	1001	HEA	C3C-C2C-C1C	-5.19	100.89	107.16
5	A	1001	HEA	CHA-C4D-ND	-5.15	118.82	124.42
5	E	1002	HEA	C2D-C1D-ND	5.04	115.81	109.84
5	A	1002	HEA	C4A-NA-C1A	-5.04	100.42	105.35
5	E	1002	HEA	C4A-NA-C1A	-4.87	100.58	105.35
5	E	1002	HEA	C2C-C1C-NC	4.84	117.45	110.08
5	E	1001	HEA	C3B-C4B-NB	4.74	115.45	109.84
5	A	1001	HEA	C3B-C4B-NB	4.68	115.38	109.84
5	A	1002	HEA	C2C-C1C-NC	4.62	117.12	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1002	HEA	C3A-C2A-C1A	-4.57	102.71	107.08
5	E	1001	HEA	C2D-C1D-ND	4.41	115.07	109.84
5	E	1001	HEA	C2C-C1C-NC	4.36	116.73	110.08
5	A	1001	HEA	C2B-C1B-NB	4.35	115.10	109.88
5	A	1001	HEA	C2A-C1A-NA	4.33	114.54	110.32
5	A	1001	HEA	C3A-C2A-C1A	-4.30	102.97	107.08
5	A	1002	HEA	CHA-C1A-NA	-4.23	119.86	124.44
5	A	1002	HEA	C1D-C2D-C3D	-4.23	102.51	106.96
5	E	1002	HEA	C1B-C2B-C3B	-4.18	101.80	106.80
5	E	1001	HEA	C2A-C1A-NA	4.18	114.39	110.32
5	A	1001	HEA	C2D-C1D-ND	4.10	114.70	109.84
5	A	1002	HEA	C1B-C2B-C3B	-4.08	101.92	106.80
5	E	1001	HEA	C2B-C1B-NB	4.07	114.76	109.88
5	A	1001	HEA	C1A-CHA-C4D	-4.05	117.33	126.06
5	E	1002	HEA	C3A-C2A-C1A	-4.04	103.22	107.08
5	A	1001	HEA	C2C-C1C-NC	4.04	116.23	110.08
5	E	1002	HEA	CHA-C4D-ND	-3.86	120.23	124.42
5	E	1002	HEA	CHB-C1B-NB	-3.81	120.28	124.42
5	E	1001	HEA	C3A-C2A-C1A	-3.79	103.46	107.08
5	E	1002	HEA	C1D-C2D-C3D	-3.68	103.08	106.96
5	E	1002	HEA	C4D-C3D-C2D	-3.67	101.55	106.90
7	E	1004	HQO	O1-C1-C10	3.67	120.89	116.31
5	A	1002	HEA	C13-C12-C11	-3.61	108.92	114.35
5	A	1002	HEA	CHA-C4D-ND	-3.61	120.50	124.42
7	A	1004	HQO	O1-C1-C10	3.60	120.80	116.31
5	A	1001	HEA	C1D-C2D-C3D	-3.59	103.18	106.96
5	E	1002	HEA	CHA-C1A-NA	-3.57	120.58	124.44
5	E	1001	HEA	C4D-C3D-C2D	-3.50	101.80	106.90
5	E	1001	HEA	C1A-CHA-C4D	-3.49	118.53	126.06
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	A	1001	HEA	CHB-C1B-NB	-3.45	120.67	124.42
5	E	1001	HEA	C1D-C2D-C3D	-3.45	103.33	106.96
5	E	1002	HEA	C13-C14-C15	-3.32	119.66	127.66
5	A	1002	HEA	C4D-C3D-C2D	-3.30	102.08	106.90
5	E	1001	HEA	C4A-NA-C1A	-3.27	102.15	105.35
5	A	1001	HEA	C4D-C3D-C2D	-3.26	102.15	106.90
5	E	1002	HEA	C4B-NB-C1B	-3.26	101.71	105.07
5	E	1001	HEA	C4B-C3B-C2B	-3.24	101.88	107.41
5	E	1002	HEA	C26-C15-C16	3.22	120.69	115.27
5	A	1002	HEA	CHB-C1B-NB	-3.22	120.92	124.42
5	A	1001	HEA	C1B-C2B-C3B	-3.16	103.03	106.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1002	HEA	C27-C19-C20	3.15	120.56	115.27
5	E	1001	HEA	CAD-C3D-C4D	3.13	130.12	124.66
5	A	1001	HEA	C26-C15-C16	3.12	120.53	115.27
5	A	1001	HEA	C4A-NA-C1A	-3.11	102.31	105.35
5	E	1002	HEA	CHC-C1C-C2C	-3.07	118.56	127.24
5	A	1001	HEA	C4B-C3B-C2B	-2.93	102.41	107.41
5	A	1001	HEA	C17-C18-C19	-2.88	120.73	127.66
5	E	1002	HEA	C4B-C3B-C2B	-2.87	102.51	107.41
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	CHB-C1B-NB	-2.84	121.33	124.42
5	A	1002	HEA	C4B-NB-C1B	-2.84	102.14	105.07
5	E	1002	HEA	CMB-C2B-C1B	2.82	129.33	125.04
5	A	1002	HEA	CHC-C1C-C2C	-2.81	119.30	127.24
5	E	1001	HEA	CAA-C2A-C1A	2.81	130.19	124.89
5	A	1002	HEA	CMB-C2B-C1B	2.78	129.28	125.04
5	A	1001	HEA	CMB-C2B-C1B	2.74	129.21	125.04
5	E	1001	HEA	C26-C15-C16	2.71	119.83	115.27
5	A	1002	HEA	CAA-C2A-C1A	2.70	129.98	124.89
5	A	1001	HEA	CAA-C2A-C1A	2.69	129.96	124.89
5	E	1002	HEA	C1D-ND-C4D	-2.68	102.31	105.07
5	A	1002	HEA	C25-C23-C24	2.68	120.52	114.60
5	A	1002	HEA	C1D-ND-C4D	-2.68	102.31	105.07
5	A	1002	HEA	C4B-C3B-C2B	-2.67	102.85	107.41
5	E	1001	HEA	C1B-C2B-C3B	-2.67	103.61	106.80
5	A	1002	HEA	C4C-NC-C1C	-2.63	102.77	105.35
5	E	1001	HEA	CHB-C4A-NA	-2.60	121.62	124.44
5	E	1002	HEA	C4C-NC-C1C	-2.58	102.82	105.35
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	1002	HEA	CHB-C4A-NA	-2.51	121.73	124.44
5	A	1001	HEA	C25-C23-C24	2.49	120.09	114.60
5	A	1001	HEA	CHB-C4A-NA	-2.47	121.77	124.44
5	E	1002	HEA	CAD-C3D-C4D	2.47	128.97	124.66
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	1001	HEA	CMD-C2D-C1D	2.43	128.74	125.04
5	A	1001	HEA	CAD-C3D-C4D	2.43	128.90	124.66
5	A	1002	HEA	CMD-C2D-C1D	2.38	128.67	125.04
5	E	1002	HEA	C27-C19-C20	2.38	119.28	115.27
5	A	1001	HEA	CHC-C4B-NB	-2.36	121.47	124.37
5	A	1001	HEA	CMD-C2D-C1D	2.36	128.63	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1002	HEA	CMD-C2D-C1D	2.29	128.53	125.04
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	E	1002	HEA	C1A-CHA-C4D	-2.24	121.22	126.06
5	E	1002	HEA	CMC-C2C-C3C	2.24	132.00	126.59
5	A	1001	HEA	OMA-CMA-C3A	-2.19	120.74	125.69
5	E	1001	HEA	CHC-C4B-NB	-2.16	121.71	124.37
5	A	1002	HEA	CHD-C1D-C2D	-2.14	120.78	126.73
5	A	1001	HEA	CMC-C2C-C3C	2.14	131.76	126.59
5	E	1001	HEA	CMB-C2B-C1B	2.13	128.29	125.04
5	A	1002	HEA	CAD-CBD-CGD	-2.12	109.03	113.60
5	E	1001	HEA	CMC-C2C-C1C	2.11	128.58	125.37
5	A	1002	HEA	C21-C22-C23	-2.10	120.56	127.75
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	E	1002	HEA	CHD-C1D-C2D	-2.06	121.00	126.73
5	A	1002	HEA	CMC-C2C-C3C	2.04	131.52	126.59
5	A	1002	HEA	CAD-C3D-C4D	2.03	128.20	124.66

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	E	1001	HEA	C2A-C3A-CMA-OMA
5	E	1001	HEA	C4A-C3A-CMA-OMA
5	E	1001	HEA	C3B-C11-C12-C13
5	A	1001	HEA	C15-C16-C17-C18
5	E	1001	HEA	C15-C16-C17-C18
5	A	1001	HEA	O11-C11-C12-C13
5	E	1001	HEA	O11-C11-C12-C13
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	E	1002	HEA	C2D-C3D-CAD-CBD
5	A	1002	HEA	C4D-C3D-CAD-CBD
5	E	1002	HEA	C4D-C3D-CAD-CBD
5	A	1002	HEA	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
5	E	1002	HEA	C2A-C3A-CMA-OMA
5	E	1002	HEA	CAD-CBD-CGD-O1D
5	A	1002	HEA	CAD-CBD-CGD-O1D
5	A	1002	HEA	CAD-CBD-CGD-O2D
5	A	1002	HEA	C26-C15-C16-C17
5	E	1002	HEA	CAD-CBD-CGD-O2D
5	E	1002	HEA	CAA-CBA-CGA-O2A
5	A	1002	HEA	CAA-CBA-CGA-O2A
5	E	1001	HEA	CAD-CBD-CGD-O2D
5	A	1001	HEA	CAD-CBD-CGD-O2D
5	E	1002	HEA	CAA-CBA-CGA-O1A
5	E	1002	HEA	C26-C15-C16-C17
5	A	1002	HEA	CAA-CBA-CGA-O1A
5	E	1001	HEA	CAD-CBD-CGD-O1D
5	A	1001	HEA	CAD-CBD-CGD-O1D

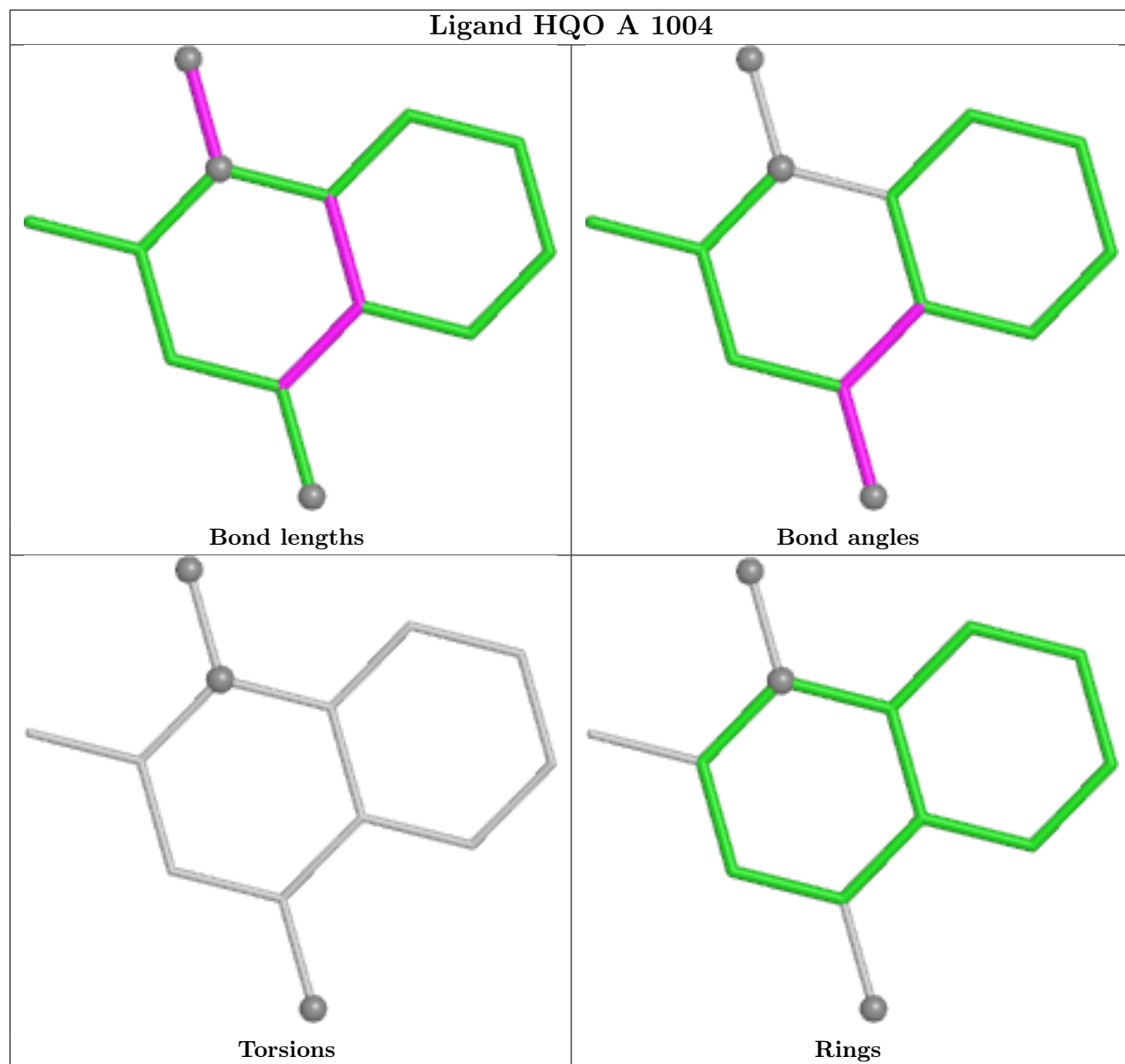
There are no ring outliers.

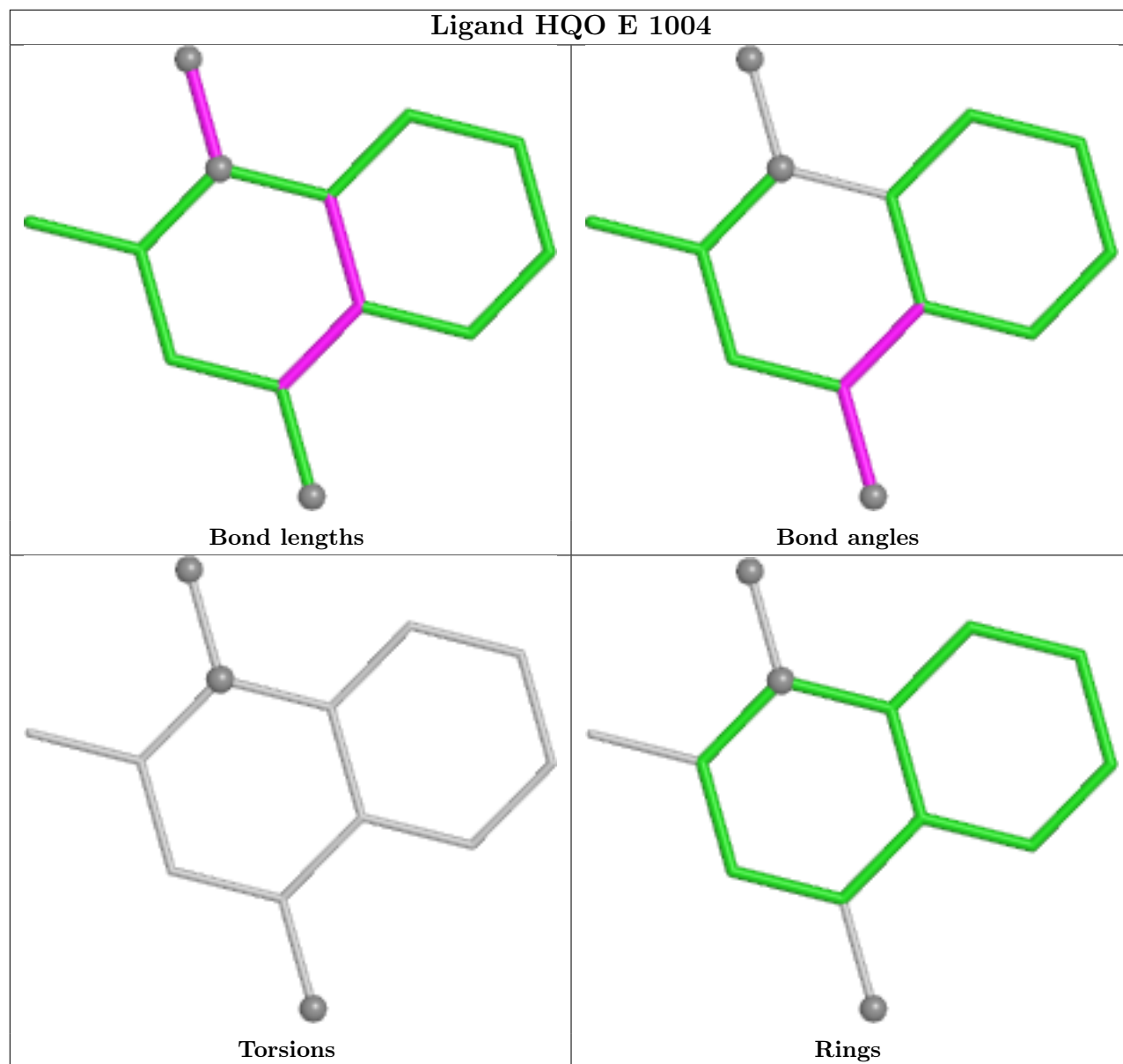
6 monomers are involved in 35 short contacts:

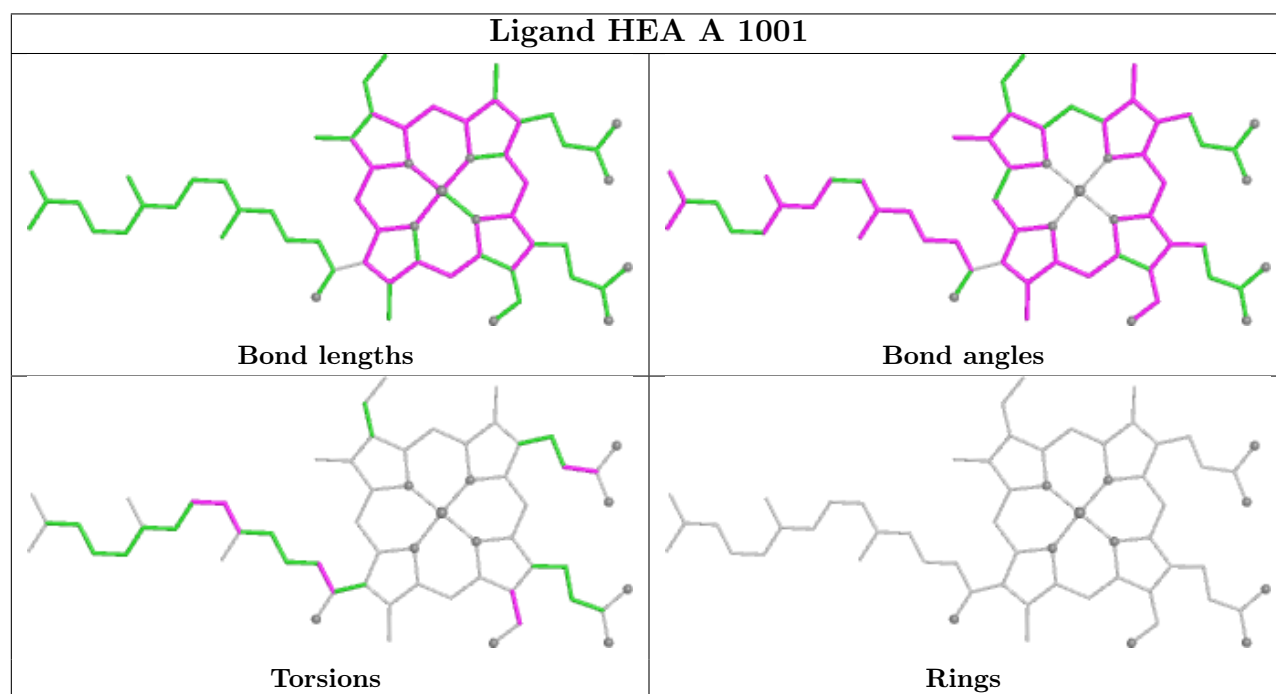
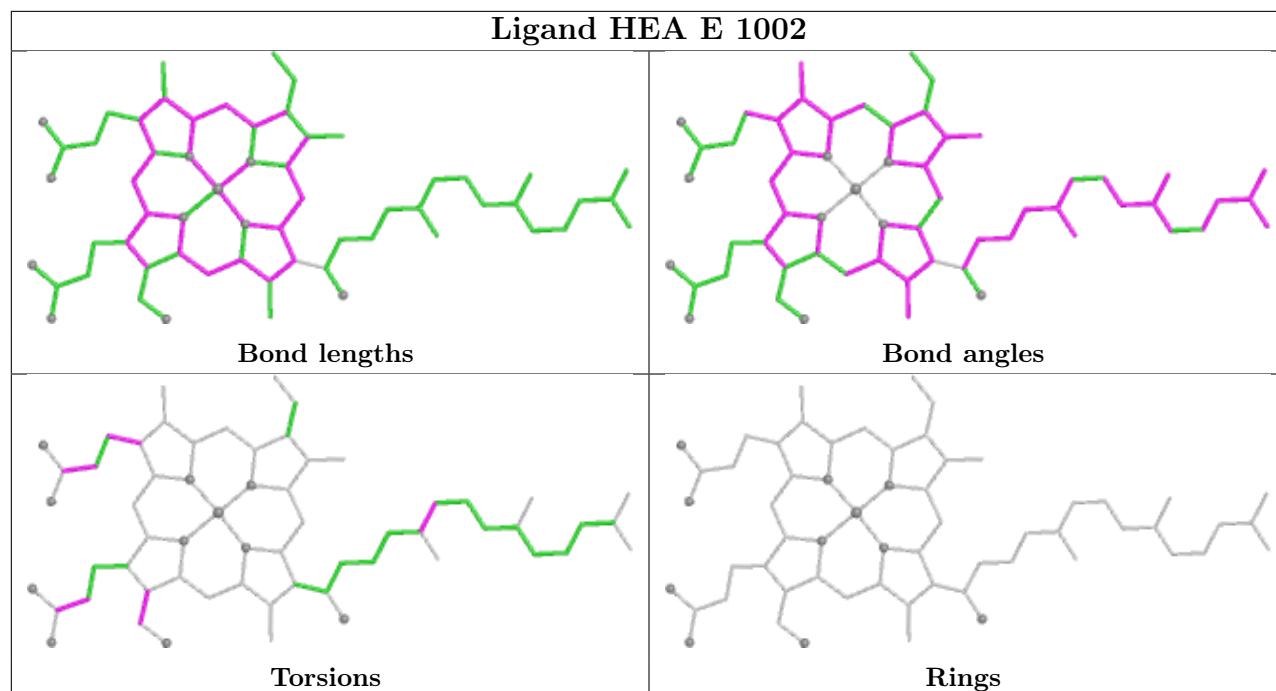
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1004	HQO	4	0
7	E	1004	HQO	5	0
5	E	1002	HEA	6	0
5	A	1001	HEA	11	0
5	E	1001	HEA	4	0
5	A	1002	HEA	5	0

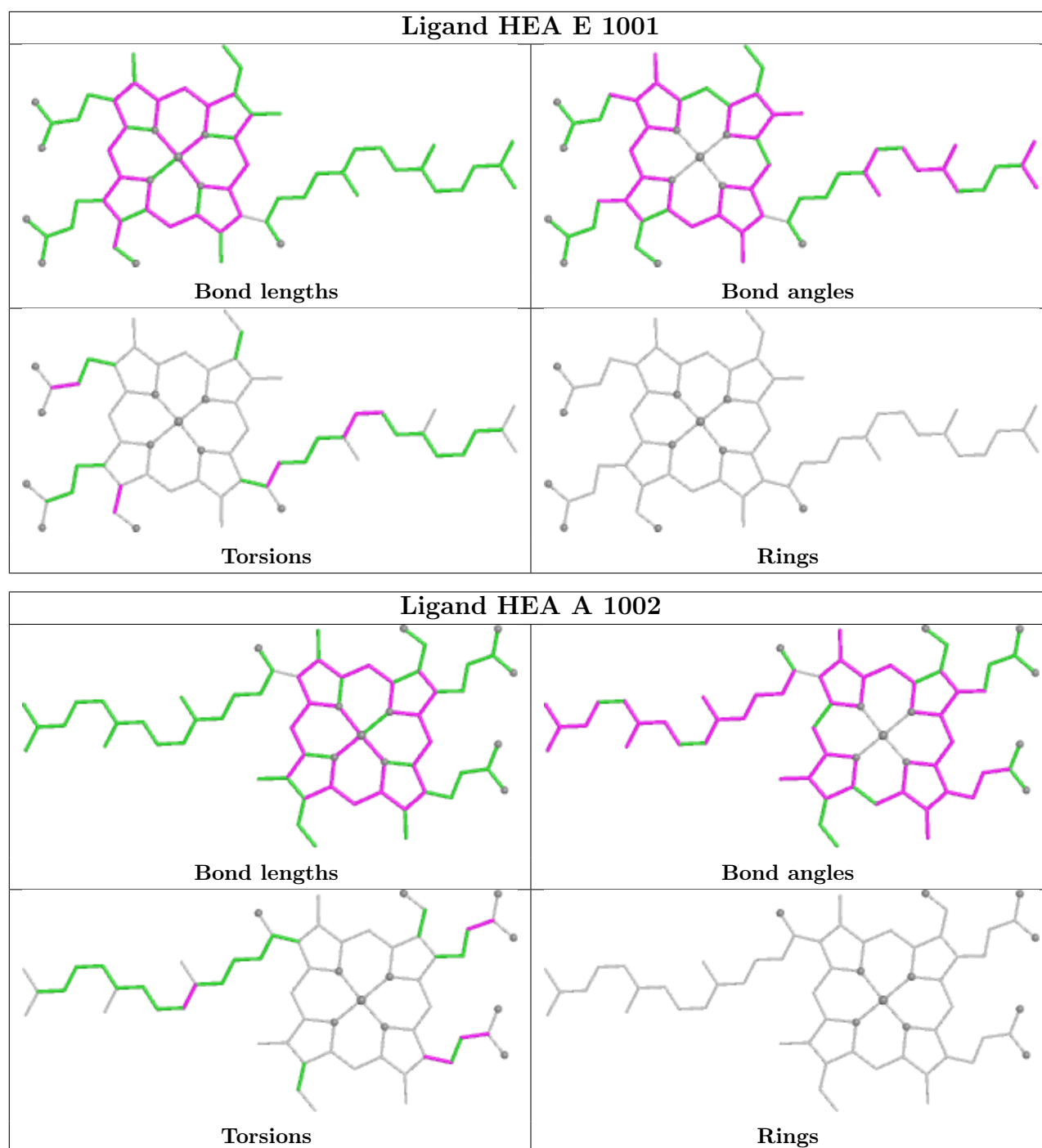
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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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%)	1.76	192 (31%)  	68, 108, 149, 180	0
1	E	607/655 (92%)	1.75	192 (31%)  	66, 111, 155, 191	0
2	B	256/296 (86%)	1.83	87 (33%)  	90, 139, 195, 223	0
2	F	256/296 (86%)	1.86	98 (38%)  	79, 134, 197, 235	0
3	C	178/204 (87%)	1.60	54 (30%)  	79, 115, 191, 235	0
3	G	178/204 (87%)	1.82	56 (31%)  	72, 124, 187, 200	0
4	D	48/124 (38%)	2.63	21 (43%)  	81, 115, 158, 166	0
4	H	48/124 (38%)	2.02	15 (31%)  	72, 109, 152, 160	0
All	All	2178/2558 (85%)	1.79	715 (32%)  	66, 117, 179, 235	0

All (715) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	274	HIS	14.5
1	A	440	PHE	12.0
1	E	405	GLN	12.0
1	A	437	PRO	11.9
1	E	333	THR	11.8
1	A	441	GLY	11.6
4	D	63	MET	11.2
3	G	144	HIS	11.1
2	B	92	SER	9.7
2	B	97	PRO	9.5
1	A	86	ASN	9.4
3	G	126	ALA	9.2
1	E	407	HIS	9.1
4	H	72	THR	8.9
3	G	53	ALA	8.4
1	E	516	SER	8.1

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Mol	Chain	Res	Type	RSRZ
4	D	69	GLU	8.0
1	A	541	SER	7.8
1	E	406	TYR	7.8
4	D	60	LEU	7.8
1	A	436	TYR	7.6
2	B	73	VAL	7.5
1	A	178	SER	7.4
3	C	102	ILE	7.4
2	F	106	LEU	7.4
2	B	95	LYS	7.3
4	D	59	LEU	7.2
1	A	542	ALA	7.2
2	F	27	PHE	7.1
1	A	314	GLY	7.1
1	A	439	MET	7.1
4	H	69	GLU	7.1
1	E	580	ILE	7.0
2	B	190	THR	6.9
2	F	107	VAL	6.9
1	A	438	LYS	6.9
1	A	432	PHE	6.7
1	E	334	MET	6.6
3	G	34	GLU	6.6
1	E	404	TYR	6.6
2	F	169	LEU	6.6
1	A	543	ILE	6.5
2	F	277	THR	6.5
1	E	618	VAL	6.5
1	A	540	SER	6.5
1	A	357	VAL	6.5
2	F	163	TYR	6.5
2	B	191	GLY	6.3
3	G	140	LEU	6.3
3	C	97	VAL	6.1
2	B	188	ASN	6.0
1	E	468	TYR	6.0
3	G	124	GLU	6.0
1	E	370	ARG	5.9
2	F	30	PHE	5.9
2	F	156	PRO	5.9
1	A	408	ASN	5.8
2	F	19	ASP	5.8

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Mol	Chain	Res	Type	RSRZ
1	E	408	ASN	5.8
1	E	441	GLY	5.8
4	D	80	PHE	5.8
1	A	478	ARG	5.7
2	B	236	ASN	5.7
1	A	52	ASP	5.7
1	E	164	ALA	5.7
2	F	23	LEU	5.7
3	C	78	SER	5.7
1	E	66	ILE	5.5
1	E	27	THR	5.5
1	A	320	SER	5.5
1	A	355	THR	5.5
3	G	143	THR	5.5
1	A	175	ASN	5.5
4	D	74	GLN	5.4
1	A	358	LYS	5.4
3	G	89	ARG	5.4
1	E	568	LYS	5.4
1	A	163	ASN	5.4
1	A	317	ILE	5.4
1	A	55	LYS	5.3
1	E	69	PHE	5.3
1	E	619	LEU	5.3
1	A	383	PHE	5.3
2	F	143	LYS	5.3
1	A	416	PHE	5.2
1	E	191	GLN	5.2
2	B	271	VAL	5.2
3	G	181	TYR	5.2
1	A	458	ILE	5.2
1	E	211	MET	5.2
1	A	179	PRO	5.2
2	B	98	GLU	5.2
4	H	63	MET	5.2
1	E	63	SER	5.2
2	B	187	ALA	5.1
4	H	70	ASN	5.1
4	D	77	ASN	5.0
2	B	275	SER	5.0
1	A	384	ILE	5.0
1	E	247	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
1	E	514	TYR	5.0
3	C	74	LEU	5.0
2	B	270	ALA	4.9
2	B	34	VAL	4.9
4	H	80	PHE	4.9
1	E	305	GLN	4.9
1	E	392	VAL	4.9
2	B	41	ILE	4.9
3	C	81	CYS	4.8
1	E	172	LEU	4.8
3	G	55	GLY	4.8
1	A	388	VAL	4.8
1	A	430	ALA	4.8
3	G	52	THR	4.8
1	E	244	VAL	4.8
1	E	29	ALA	4.8
1	A	579	LYS	4.7
1	A	172	LEU	4.7
1	A	469	PHE	4.7
1	E	332	PHE	4.7
3	C	28	TRP	4.7
2	B	17	GLN	4.7
1	E	510	CYS	4.6
1	E	95	TYR	4.6
4	H	71	GLY	4.6
2	F	159	GLY	4.6
1	A	407	HIS	4.6
1	A	58	ILE	4.6
3	C	181	TYR	4.6
1	E	615	LEU	4.6
1	A	405	GLN	4.5
2	B	277	THR	4.5
1	E	269	MET	4.5
3	G	94	LYS	4.5
1	A	47	TRP	4.5
2	F	253	GLY	4.5
4	D	78	THR	4.5
1	E	622	MET	4.5
3	G	90	ARG	4.5
1	E	212	ARG	4.4
2	F	109	TYR	4.4
2	B	165	MET	4.4

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Mol	Chain	Res	Type	RSRZ
2	F	168	MET	4.4
1	A	362	TRP	4.4
3	C	106	LEU	4.4
2	B	154	TRP	4.3
2	B	16	GLN	4.3
2	B	276	LYS	4.3
1	E	248	LEU	4.3
1	A	619	LEU	4.3
3	C	62	PHE	4.3
3	G	39	SER	4.3
1	E	210	LYS	4.3
3	G	54	GLY	4.3
1	E	583	PRO	4.3
1	E	630	ASP	4.3
1	A	480	TYR	4.3
3	C	61	LEU	4.3
1	A	137	LEU	4.2
2	F	158	LEU	4.2
1	A	14	PRO	4.2
3	C	180	LEU	4.2
3	G	146	THR	4.2
1	A	454	TRP	4.2
2	B	259	ALA	4.2
1	A	275	PHE	4.2
1	A	61	ILE	4.2
3	G	35	ILE	4.2
1	E	105	ILE	4.2
3	G	32	GLY	4.1
1	E	33	VAL	4.1
2	B	50	LYS	4.1
2	B	36	PHE	4.1
1	A	321	VAL	4.1
1	E	412	LEU	4.1
1	A	318	ALA	4.1
1	A	166	TRP	4.1
1	A	359	ILE	4.1
3	C	80	THR	4.1
1	A	386	ASN	4.1
1	A	356	GLY	4.0
1	E	478	ARG	4.0
2	F	115	TRP	4.0
1	A	96	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	381	LEU	4.0
1	E	631	ASN	4.0
1	E	314	GLY	4.0
1	E	633	TYR	3.9
4	D	90	LEU	3.9
1	E	166	TRP	3.9
1	A	385	PRO	3.9
1	A	88	SER	3.9
1	E	584	SER	3.9
2	F	141	LEU	3.9
2	B	235	GLU	3.9
3	C	149	THR	3.9
1	A	578	LYS	3.9
1	E	504	VAL	3.9
1	E	566	GLU	3.9
2	F	161	GLN	3.9
1	A	510	CYS	3.9
3	C	71	THR	3.9
2	B	166	ALA	3.9
1	A	618	VAL	3.9
1	A	507	LEU	3.8
3	G	189	TRP	3.8
2	B	131	TYR	3.8
2	B	279	PRO	3.8
2	F	108	VAL	3.8
1	A	435	TRP	3.8
3	G	114	GLU	3.8
3	G	147	HIS	3.8
2	F	190	THR	3.8
2	F	44	VAL	3.8
1	A	167	THR	3.7
1	E	507	LEU	3.7
1	A	486	ASP	3.7
1	E	67	MET	3.7
2	B	195	ALA	3.7
3	G	36	VAL	3.7
1	A	91	ASP	3.7
4	H	67	GLU	3.7
1	A	546	HIS	3.7
2	F	274	HIS	3.7
2	B	96	ALA	3.7
2	F	78	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
3	G	125	GLY	3.7
2	F	165	MET	3.7
3	C	63	GLU	3.7
4	D	88	ILE	3.6
2	F	20	LEU	3.6
1	A	92	SER	3.6
2	F	275	SER	3.6
3	G	134	TRP	3.6
1	A	296	GLU	3.6
1	A	269	MET	3.6
2	F	250	VAL	3.6
2	B	192	GLU	3.6
2	B	285	LYS	3.6
1	A	276	TRP	3.6
1	A	164	ALA	3.6
1	A	380	ALA	3.6
1	A	15	LEU	3.6
1	E	530	GLY	3.6
1	A	622	MET	3.6
1	A	477	ARG	3.6
2	F	237	VAL	3.6
1	A	379	TRP	3.5
2	B	257	GLU	3.5
1	E	194	GLY	3.5
4	D	95	ILE	3.5
2	B	152	SER	3.5
2	F	142	PHE	3.5
3	C	105	LEU	3.5
1	A	476	PRO	3.5
1	E	263	GLU	3.5
1	A	225	THR	3.5
1	E	331	PHE	3.4
2	F	150	MET	3.4
1	E	411	PHE	3.4
1	A	583	PRO	3.4
1	E	34	LEU	3.4
2	F	259	ALA	3.4
3	G	127	ALA	3.4
1	E	567	GLU	3.4
1	E	70	ARG	3.4
1	A	238	ALA	3.4
2	F	34	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
2	F	193	HIS	3.4
1	A	474	GLY	3.4
1	E	423	GLY	3.4
4	H	81	GLY	3.4
3	G	171	THR	3.4
2	F	154	TRP	3.4
1	E	472	LEU	3.4
1	A	138	ASN	3.4
1	A	387	PHE	3.4
1	E	103	GLY	3.4
1	E	62	ILE	3.4
4	H	79	LEU	3.4
1	E	240	PRO	3.4
1	E	268	PRO	3.4
1	A	136	TYR	3.4
1	A	327	TRP	3.3
1	A	264	ALA	3.3
2	B	273	PRO	3.3
3	G	138	PHE	3.3
1	E	442	HIS	3.3
1	E	570	GLU	3.3
3	G	145	GLY	3.3
1	E	582	MET	3.3
2	B	234	PRO	3.3
2	B	225	LYS	3.3
2	F	269	GLN	3.3
1	E	196	GLY	3.3
1	E	35	THR	3.3
1	A	442	HIS	3.3
1	E	486	ASP	3.3
2	F	251	ASP	3.3
2	F	189	PHE	3.3
4	D	72	THR	3.3
1	E	609	TRP	3.2
1	E	107	ILE	3.2
1	E	235	ILE	3.2
1	A	176	ASP	3.2
2	F	236	ASN	3.2
1	A	62	ILE	3.2
2	F	149	SER	3.2
1	E	161	SER	3.2
1	A	85	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	434	PHE	3.2
1	E	480	TYR	3.2
1	E	178	SER	3.2
2	B	156	PRO	3.2
2	B	266	LEU	3.2
1	E	440	PHE	3.1
4	D	70	ASN	3.1
1	E	157	VAL	3.1
2	B	70	VAL	3.1
1	A	409	THR	3.1
2	B	178	LYS	3.1
1	A	139	ASN	3.1
2	B	186	ASN	3.1
2	F	258	TYR	3.1
2	B	37	VAL	3.1
2	F	252	HIS	3.1
1	A	57	GLY	3.1
2	B	150	MET	3.1
2	F	172	GLN	3.1
3	C	98	ILE	3.1
2	F	28	MET	3.1
1	E	128	GLY	3.1
2	F	160	GLY	3.1
1	A	93	ASN	3.1
1	E	537	TRP	3.1
1	E	169	TYR	3.1
2	F	257	GLU	3.1
1	E	393	THR	3.1
1	A	173	ALA	3.1
1	A	580	ILE	3.1
1	E	479	ILE	3.1
1	E	296	GLU	3.1
3	C	153	PHE	3.1
3	C	70	MET	3.1
1	E	90	LEU	3.1
3	G	57	LEU	3.1
3	G	142	GLY	3.1
2	B	162	LYS	3.0
3	G	82	GLY	3.0
1	A	453	PHE	3.0
1	E	64	ALA	3.0
1	E	255	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	428	CYS	3.0
2	F	153	LEU	3.0
2	F	192	GLU	3.0
1	E	544	PRO	3.0
3	G	151	GLY	3.0
3	C	146	THR	3.0
1	A	174	SER	3.0
1	E	416	PHE	3.0
1	A	177	MET	3.0
3	G	50	ASN	3.0
1	E	421	ILE	3.0
2	B	31	ILE	3.0
2	B	93	LEU	3.0
3	C	53	ALA	3.0
2	F	22	LEU	3.0
1	E	65	VAL	3.0
4	D	61	MET	3.0
3	G	21	ARG	2.9
3	G	40	THR	2.9
4	D	92	SER	2.9
3	G	197	TYR	2.9
3	C	34	GLU	2.9
3	G	172	SER	2.9
1	A	382	ALA	2.9
2	F	134	ILE	2.9
2	B	46	TYR	2.9
1	E	32	PHE	2.9
1	E	106	MET	2.9
1	E	477	ARG	2.9
1	A	555	VAL	2.9
3	G	148	VAL	2.9
1	E	15	LEU	2.9
1	E	482	TYR	2.9
2	F	194	PHE	2.9
3	C	171	THR	2.9
2	B	262	ALA	2.9
3	G	118	PHE	2.9
2	F	260	MET	2.9
1	E	352	SER	2.9
1	E	613	VAL	2.9
3	C	96	VAL	2.9
3	C	172	SER	2.9

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Mol	Chain	Res	Type	RSRZ
3	G	119	VAL	2.9
1	E	264	ALA	2.9
4	H	53	ILE	2.9
1	E	465	PHE	2.9
1	E	476	PRO	2.9
2	F	268	TYR	2.9
2	F	285	LYS	2.9
1	E	625	ARG	2.8
3	C	77	SER	2.8
1	E	293	ILE	2.8
1	E	224	PHE	2.8
1	A	169	TYR	2.8
1	A	298	ILE	2.8
1	E	174	SER	2.8
1	E	209	LEU	2.8
2	B	42	ILE	2.8
2	B	261	GLU	2.8
3	C	27	PHE	2.8
1	A	609	TRP	2.8
1	A	535	LEU	2.8
1	A	392	VAL	2.8
1	E	92	SER	2.8
1	E	372	SER	2.8
1	E	175	ASN	2.8
1	A	311	ALA	2.8
1	E	616	ILE	2.8
2	F	31	ILE	2.8
1	E	419	VAL	2.8
2	B	201	VAL	2.8
1	A	282	GLU	2.8
1	E	96	ASN	2.8
2	F	186	ASN	2.8
2	F	282	ASN	2.8
1	E	403	ASP	2.8
3	C	73	LEU	2.7
2	F	272	SER	2.7
2	B	33	GLY	2.7
2	B	167	GLY	2.7
2	F	16	GLN	2.7
2	F	197	GLN	2.7
1	E	104	THR	2.7
1	E	481	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	485	ASN	2.7
3	C	100	THR	2.7
1	A	616	ILE	2.7
2	F	140	ILE	2.7
1	E	321	VAL	2.7
1	A	368	LYS	2.7
1	E	222	PRO	2.7
2	F	276	LYS	2.7
1	E	56	LEU	2.7
2	F	233	LEU	2.7
3	C	127	ALA	2.7
2	F	144	ILE	2.7
1	E	53	HIS	2.7
2	B	252	HIS	2.7
1	E	626	SER	2.7
3	G	96	VAL	2.7
1	A	268	PRO	2.7
1	A	354	PRO	2.7
1	E	415	HIS	2.7
1	E	262	LEU	2.7
1	A	473	GLN	2.7
1	A	277	ILE	2.7
1	E	31	ILE	2.7
4	H	95	ILE	2.7
3	G	130	THR	2.7
1	E	102	HIS	2.7
1	E	276	TRP	2.7
2	B	19	ASP	2.7
2	B	161	GLN	2.7
2	F	157	GLN	2.7
1	E	30	ILE	2.6
1	E	289	PRO	2.6
1	A	350	ALA	2.6
3	C	112	GLY	2.6
2	B	258	TYR	2.6
3	G	44	THR	2.6
3	G	100	THR	2.6
1	E	93	ASN	2.6
3	C	101	ILE	2.6
3	G	182	TRP	2.6
1	A	132	VAL	2.6
2	F	264	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	273	PRO	2.6
1	E	350	ALA	2.6
4	H	55	ALA	2.6
1	A	42	TRP	2.6
2	B	260	MET	2.6
1	A	294	PHE	2.6
1	A	606	GLU	2.6
1	A	24	ALA	2.6
1	A	237	PHE	2.6
1	A	481	THR	2.6
1	A	235	ILE	2.6
1	A	313	VAL	2.6
3	C	115	ILE	2.6
1	E	420	LEU	2.6
1	A	87	ASN	2.6
1	E	303	ARG	2.6
2	F	263	ARG	2.6
3	G	139	VAL	2.6
1	E	115	LEU	2.6
1	A	48	ILE	2.5
1	E	28	ILE	2.5
2	B	265	ARG	2.5
1	A	205	MET	2.5
1	E	110	MET	2.5
1	A	537	TRP	2.5
1	E	586	SER	2.5
1	A	491	LEU	2.5
2	B	282	ASN	2.5
1	A	484	PRO	2.5
1	E	281	PRO	2.5
1	E	61	ILE	2.5
1	A	322	LEU	2.5
2	B	213	VAL	2.5
2	F	32	VAL	2.5
1	E	163	ASN	2.5
2	B	197	GLN	2.5
2	B	256	ALA	2.5
1	E	182	GLY	2.5
4	D	66	THR	2.5
1	E	515	TYR	2.5
4	H	57	LEU	2.5
1	A	121	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	54	LYS	2.5
1	A	240	PRO	2.5
1	A	281	PRO	2.5
3	G	93	LEU	2.5
1	E	237	PHE	2.5
2	B	39	PHE	2.5
4	H	83	PHE	2.5
1	A	75	GLY	2.5
1	E	325	LEU	2.5
1	E	243	THR	2.5
1	A	342	SER	2.5
4	D	89	VAL	2.5
2	F	164	ALA	2.4
2	F	171	ASP	2.4
1	E	213	THR	2.4
2	B	20	LEU	2.4
2	B	23	LEU	2.4
2	F	174	LEU	2.4
3	G	37	LEU	2.4
2	B	269	GLN	2.4
1	E	223	MET	2.4
2	F	100	THR	2.4
3	G	56	VAL	2.4
2	F	187	ALA	2.4
3	G	99	TRP	2.4
1	A	447	ARG	2.4
3	C	189	TRP	2.4
1	A	449	GLY	2.4
2	F	234	PRO	2.4
3	C	107	GLY	2.4
1	E	22	SER	2.4
2	B	32	VAL	2.4
2	F	86	THR	2.4
3	C	143	THR	2.4
2	B	48	ASP	2.4
1	A	482	TYR	2.4
1	A	263	GLU	2.4
1	E	546	HIS	2.4
1	E	376	PRO	2.4
2	F	162	LYS	2.4
2	B	18	SER	2.4
1	A	353	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	283	VAL	2.4
1	A	560	ALA	2.4
2	F	110	ALA	2.4
2	F	105	PRO	2.3
1	E	130	ARG	2.3
2	F	249	TYR	2.3
2	B	94	GLU	2.3
1	A	352	SER	2.3
1	A	433	ILE	2.3
1	A	553	PRO	2.3
2	B	38	LEU	2.3
2	F	198	GLU	2.3
2	F	278	ASP	2.3
1	A	208	ILE	2.3
1	A	505	GLY	2.3
1	A	488	TRP	2.3
3	C	88	MET	2.3
1	A	558	GLN	2.3
1	E	369	GLY	2.3
4	D	64	HIS	2.3
1	E	461	ASN	2.3
2	B	49	ARG	2.3
2	F	185	ARG	2.3
1	E	238	ALA	2.3
1	E	298	ILE	2.3
1	E	402	ALA	2.3
1	A	126	GLN	2.3
1	A	171	PRO	2.3
1	E	131	ASP	2.3
1	E	531	VAL	2.3
1	E	587	GLY	2.3
2	F	26	GLY	2.3
1	A	461	ASN	2.3
1	E	273	ASN	2.3
2	B	246	HIS	2.3
3	C	90	ARG	2.3
1	A	325	LEU	2.3
1	E	381	LEU	2.3
1	E	434	PHE	2.3
1	E	500	PHE	2.3
3	C	163	LYS	2.3
3	C	168	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	76	ILE	2.2
4	H	50	PHE	2.2
1	A	443	LYS	2.2
1	A	222	PRO	2.2
1	E	388	VAL	2.2
3	C	82	GLY	2.2
1	A	306	LEU	2.2
3	C	52	THR	2.2
3	G	74	LEU	2.2
1	A	512	ASN	2.2
1	E	272	ALA	2.2
1	A	63	SER	2.2
1	A	323	SER	2.2
1	E	18	GLY	2.2
1	E	611	GLY	2.2
3	C	125	GLY	2.2
3	G	103	THR	2.2
1	E	116	ILE	2.2
1	E	277	ILE	2.2
1	A	307	PHE	2.2
1	E	80	ALA	2.2
1	E	565	LYS	2.2
3	G	170	GLN	2.2
4	D	58	GLN	2.2
3	C	92	SER	2.2
1	A	233	VAL	2.2
1	A	236	VAL	2.2
2	F	261	GLU	2.2
3	G	24	ILE	2.2
1	A	271	TRP	2.2
2	B	157	GLN	2.2
3	C	111	VAL	2.2
3	G	27	PHE	2.2
1	A	128	GLY	2.2
2	F	90	ILE	2.2
3	C	150	ILE	2.2
1	A	291	PHE	2.2
2	B	45	LYS	2.2
1	A	334	MET	2.2
1	A	538	ALA	2.1
1	E	290	ALA	2.1
1	E	311	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	283	VAL	2.1
3	C	148	VAL	2.1
1	A	159	GLY	2.1
1	A	194	GLY	2.1
1	E	460	PHE	2.1
2	F	191	GLY	2.1
1	A	249	LEU	2.1
1	A	366	MET	2.1
1	E	83	ALA	2.1
2	F	262	ALA	2.1
1	A	536	ASP	2.1
1	E	195	ILE	2.1
1	E	317	ILE	2.1
2	F	25	ILE	2.1
1	E	278	TRP	2.1
1	E	488	TRP	2.1
1	E	574	GLU	2.1
1	A	262	LEU	2.1
1	A	378	LEU	2.1
3	C	50	ASN	2.1
3	C	184	PHE	2.1
3	G	163	LYS	2.1
1	E	327	TRP	2.1
1	A	412	LEU	2.1
2	F	40	THR	2.1
1	E	79	ARG	2.1
1	A	290	ALA	2.1
1	A	550	ALA	2.1
1	A	455	ILE	2.1
2	F	188	ASN	2.1
2	B	193	HIS	2.1
2	F	114	ASP	2.1
1	A	71	GLY	2.1
1	A	219	MET	2.1
1	A	501	MET	2.1
1	E	628	GLU	2.1
3	C	130	THR	2.1
1	A	273	ASN	2.1
2	F	254	GLN	2.1
1	E	620	LEU	2.1
1	A	284	TYR	2.1
1	E	335	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	536	ASP	2.1
2	B	65	THR	2.1
3	C	132	ALA	2.1
1	A	360	PHE	2.1
1	A	456	PHE	2.1
1	E	87	ASN	2.1
1	A	423	GLY	2.0
1	A	431	GLY	2.0
2	B	91	TYR	2.0
2	B	115	TRP	2.0
2	B	200	ASP	2.0
2	B	255	ASP	2.0
4	D	94	TRP	2.0
2	F	94	GLU	2.0
1	E	111	ALA	2.0
2	F	280	PHE	2.0
3	C	72	PHE	2.0
3	C	133	PHE	2.0
1	E	203	ASN	2.0
4	D	91	GLY	2.0
2	B	263	ARG	2.0
2	F	238	ASP	2.0
1	A	557	SER	2.0
2	F	173	TYR	2.0
1	A	429	PHE	2.0
1	E	306	LEU	2.0
3	C	87	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

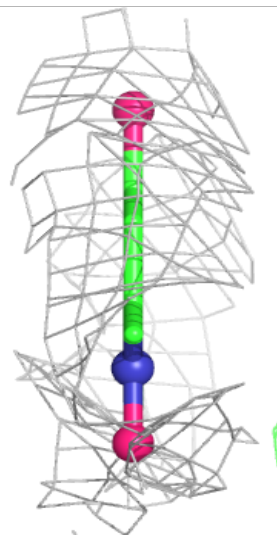
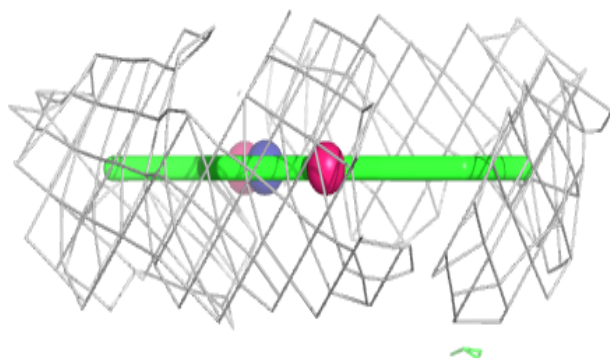
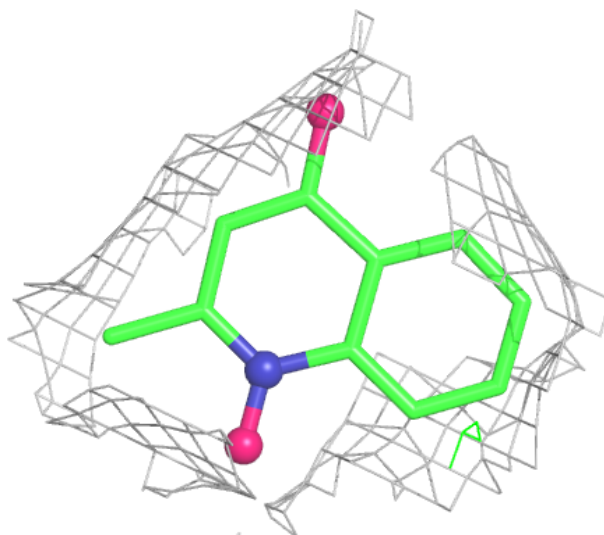
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	HQO	A	1004	13/19	0.76	0.15	95,102,107,110	0
7	HQO	E	1004	13/19	0.87	0.15	102,107,111,114	0
5	HEA	A	1002	60/60	0.89	0.31	96,118,163,168	0
5	HEA	E	1002	60/60	0.90	0.27	92,117,141,142	0
5	HEA	A	1001	60/60	0.90	0.25	91,112,132,134	0
5	HEA	E	1001	60/60	0.90	0.27	88,109,131,135	0
6	CU	E	1003	1/1	0.92	0.12	104,104,104,104	0
6	CU	A	1003	1/1	0.93	0.11	109,109,109,109	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.

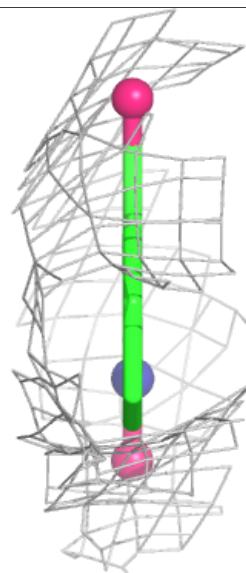
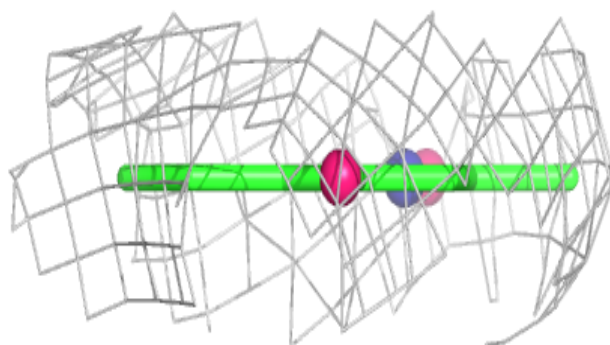
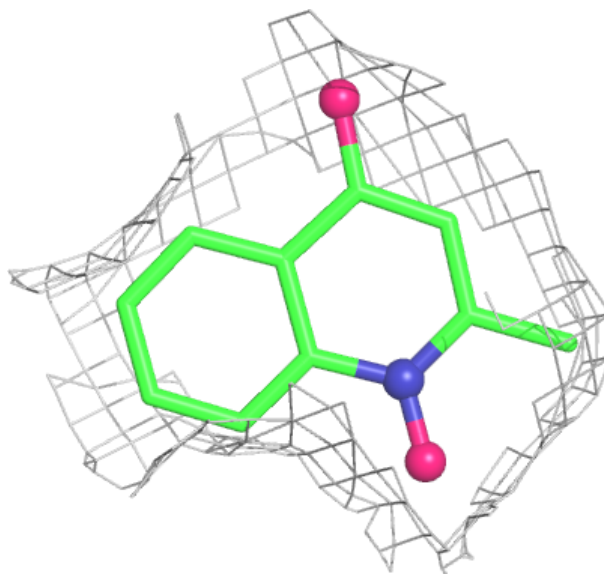
Electron density around HQO A 1004:

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



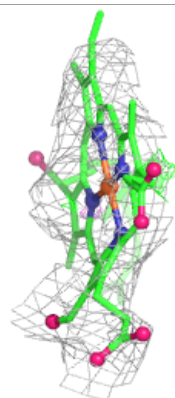
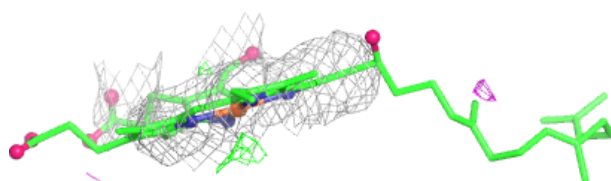
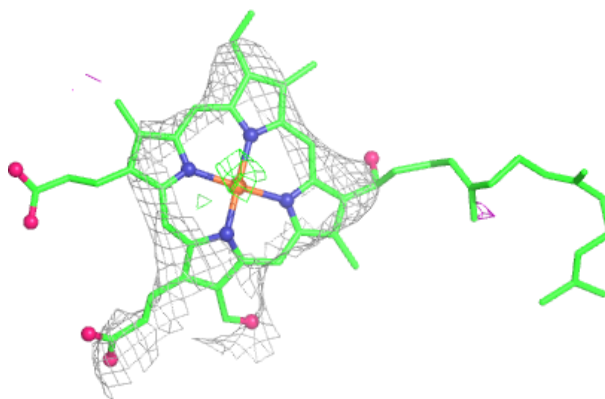
Electron density around HQO E 1004:

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

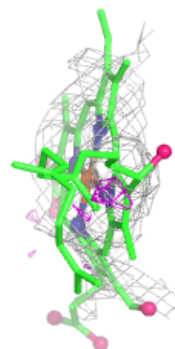
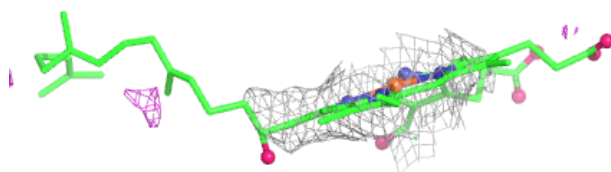
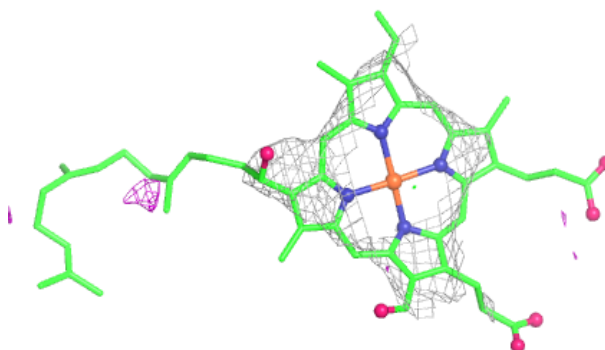


Electron density around HEA A 1002:

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

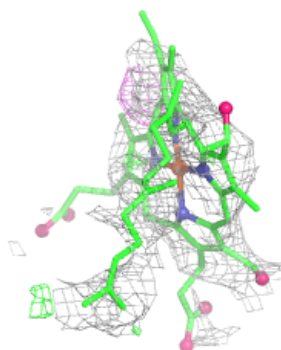
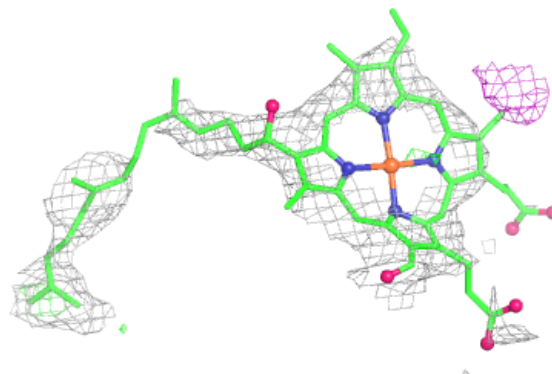
**Electron density around HEA E 1002:**

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

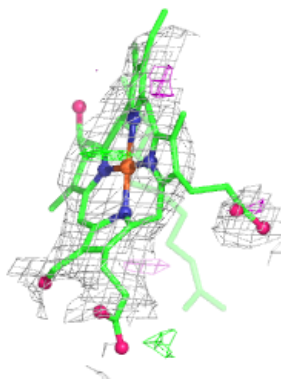
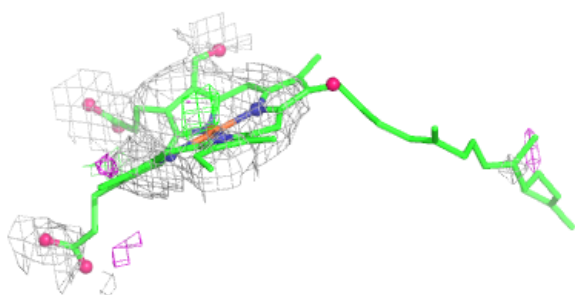
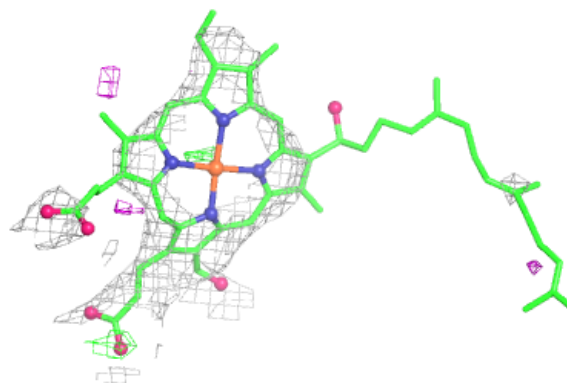


Electron density around HEA A 1001:

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

**Electron density around HEA E 1001:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.