Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 04:16 PM JST

PDB ID	:	6KOB / pdb_00006kob
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	:	3.60 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 (i) 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 (i)) were used in the production of this report:

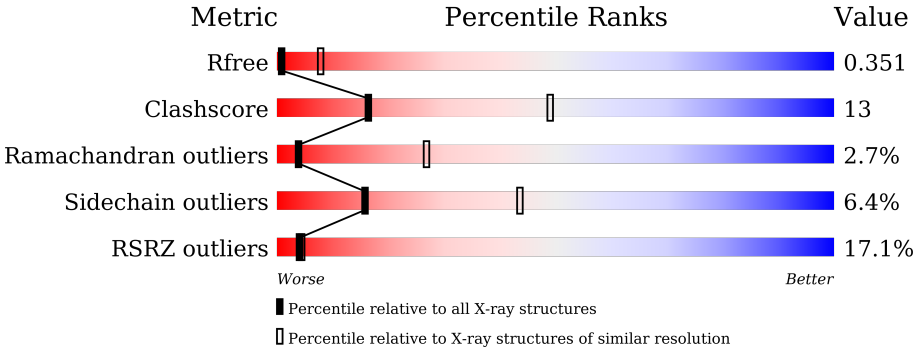
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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 (i)

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

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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 <=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	13% 62% 27% • 7%
1	E	655	19% 60% 29% • 7%
2	B	296	15% 52% 29% 6% 14%
2	F	296	16% 48% 32% 6% 14%
3	C	204	11% 67% 18% • 13%
3	G	204	14% 65% 21% • 13%

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Mol	Chain	Length	Quality of chain
4	D	124	6% 44% 11% • 44%
4	H	124	9% 47% 9% • 44%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17944 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called AA3-600 quinol oxidase subunit I.

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

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
			Total	C	N	O	S			
2	B	256	2073	1348	328	390	7	0	0	0
2	F	256	2073	1348	328	390	7	0	0	0

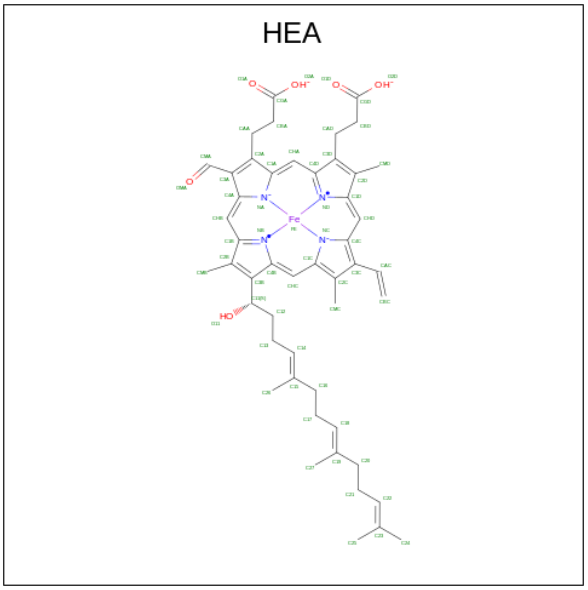
- Molecule 3 is a protein called AA3-600 quinol oxidase subunit IIII.

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

- Molecule 4 is a protein called AA3-600 quinol oxidase subunit IV,Quinol oxidase subunit 4.

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

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

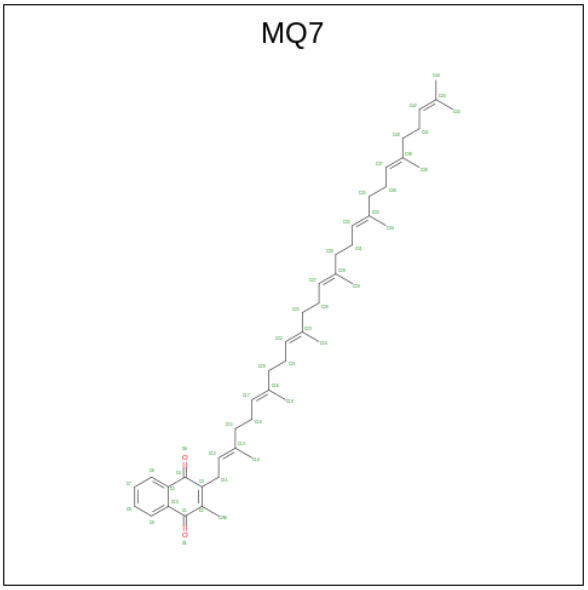


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	A	1	60	49	1	4	6	0	0
5	A	1	60	49	1	4	6	0	0
5	E	1	60	49	1	4	6	0	0
5	E	1	60	49	1	4	6	0	0

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

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

- Molecule 7 is MENAQUINONE-7 (CCD ID: MQ7) (formula: $C_{46}H_{64}O_2$).



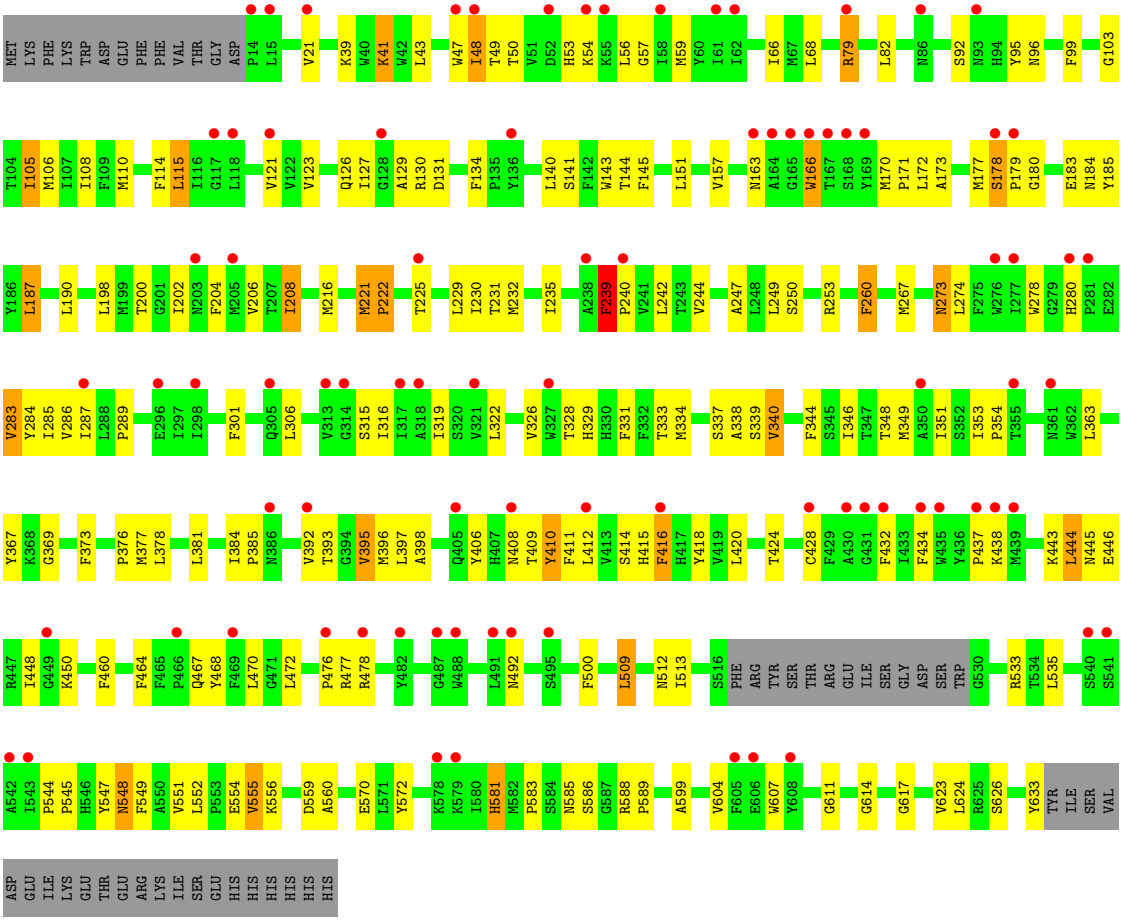
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	30	28	2	0	0
			Total	C	O		
7	E	1	30	28	2	0	0

3 Residue-property plots (i)

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

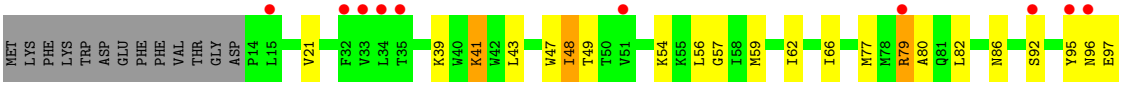
- Molecule 1: AA3-600 quinol oxidase subunit I

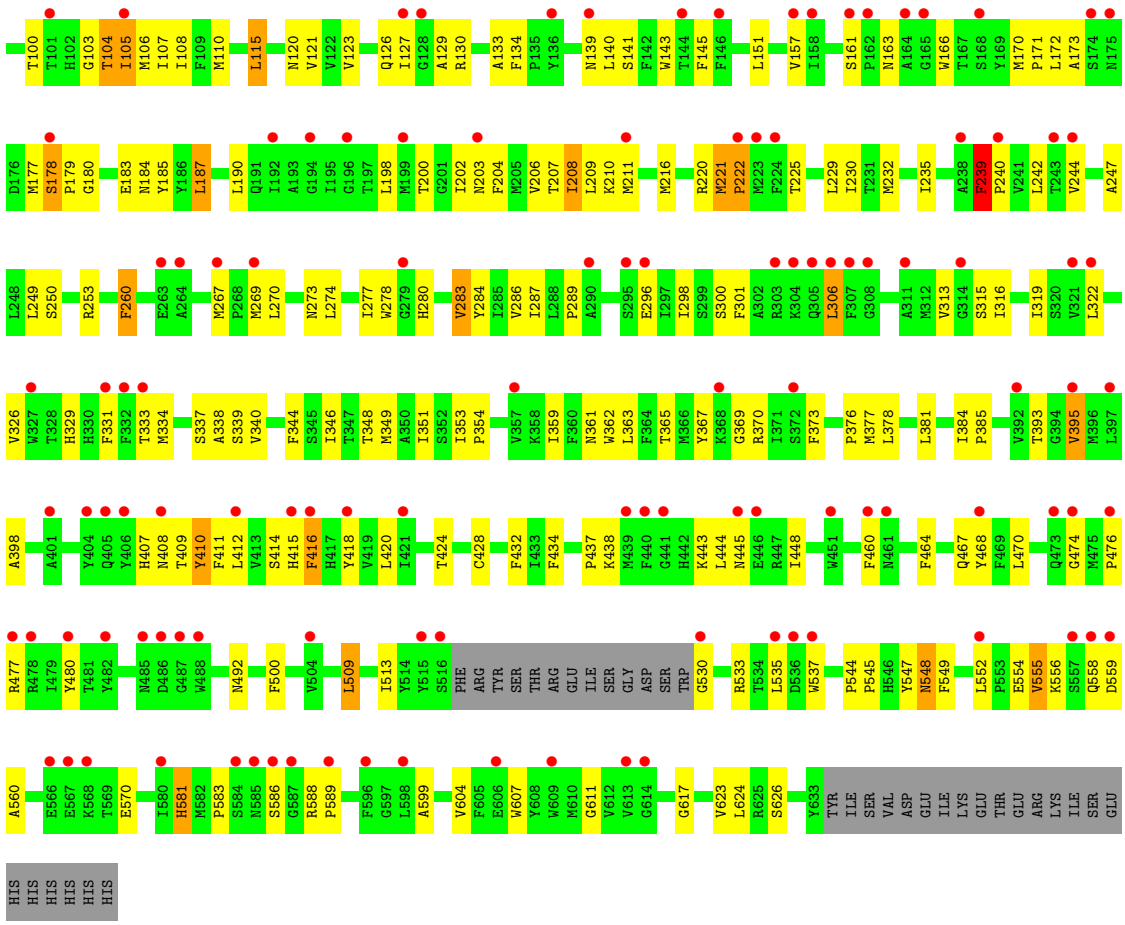
Chain A:



- Molecule 1: AA3-600 quinol oxidase subunit I

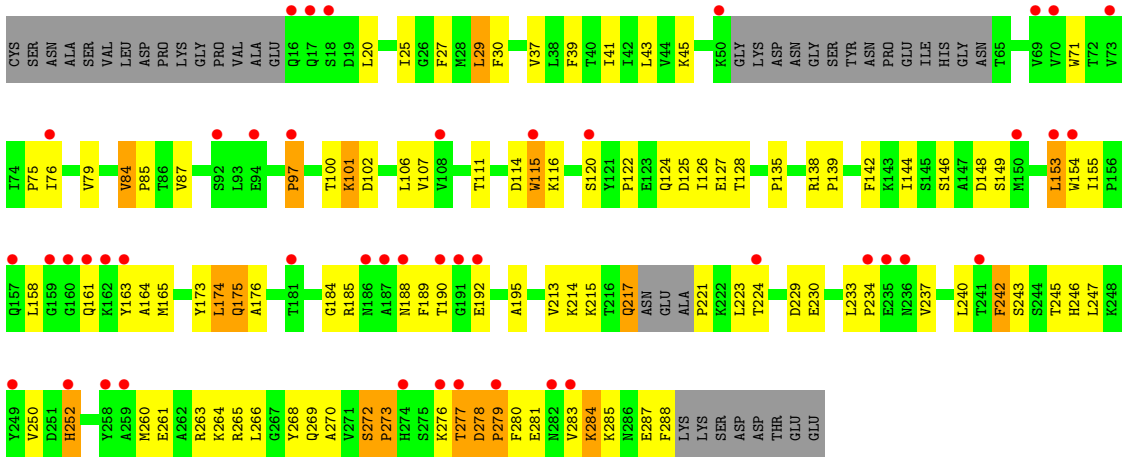
Chain E:





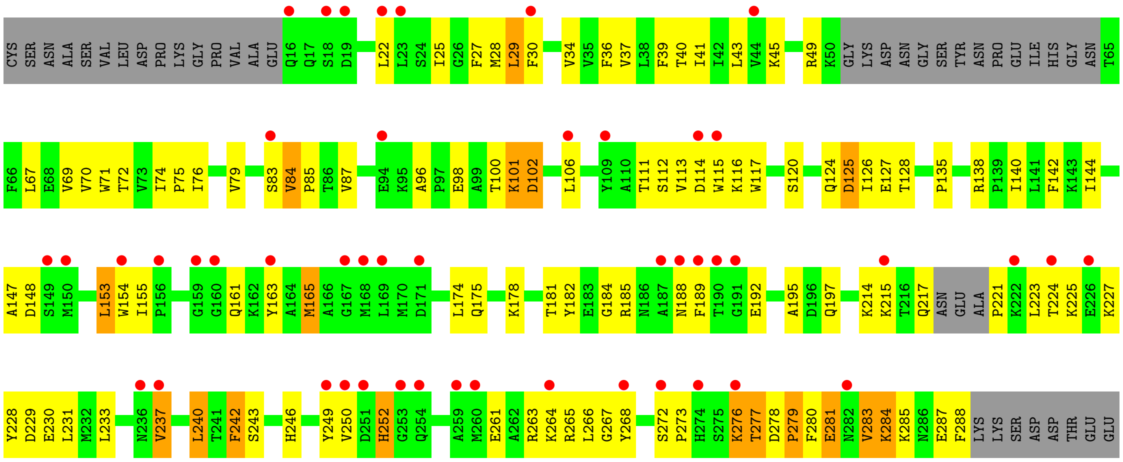
- Molecule 2: Quinol oxidase subunit 2

Chain B:



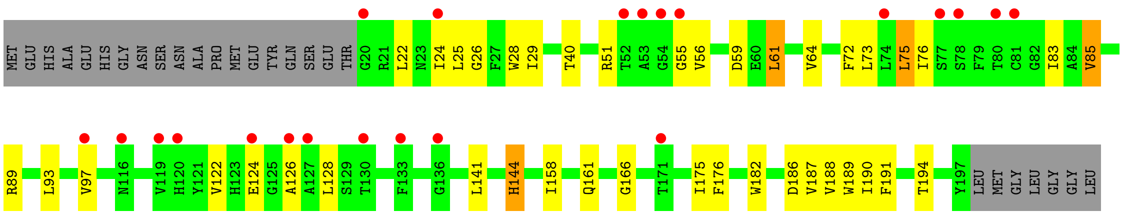
- Molecule 2: Quinol oxidase subunit 2

Chain F:



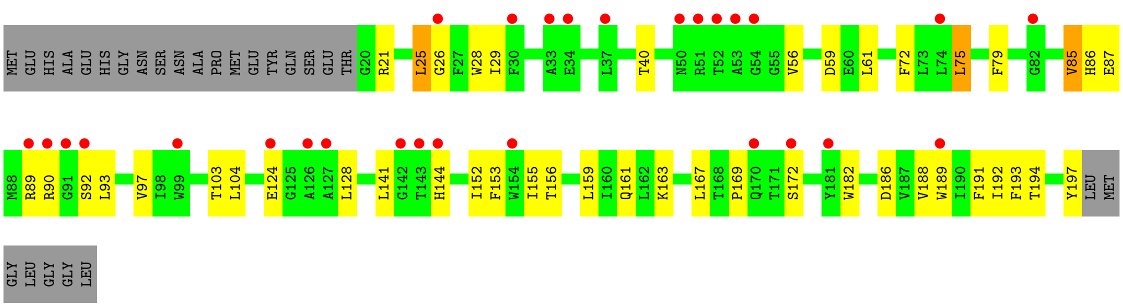
- Molecule 3: AA3-600 quinol oxidase subunit IIII

Chain C:



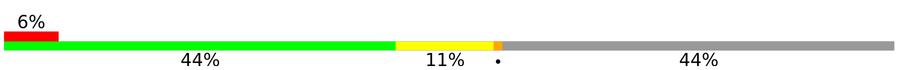
- Molecule 3: AA3-600 quinol oxidase subunit IIII

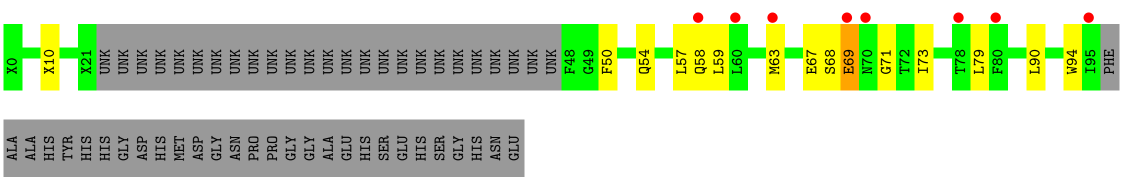
Chain G:



- Molecule 4: AA3-600 quinol oxidase subunit IV,Quinol oxidase subunit 4

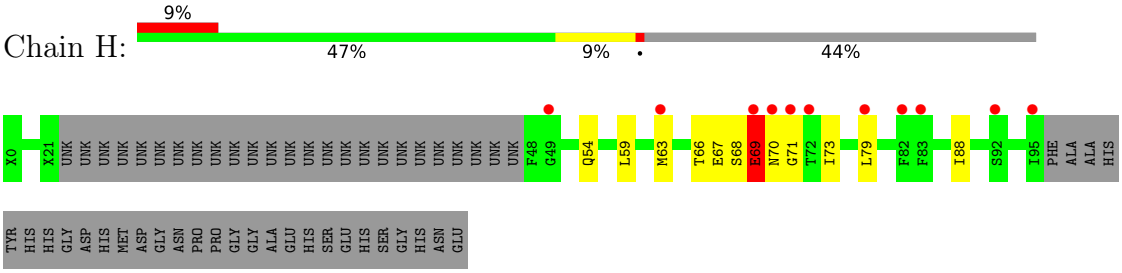
Chain D:





- Molecule 4: AA3-600 quinol oxidase subunit IV,Quinol oxidase subunit 4

Chain H:


9%
47%
9%
44%
X0 X21 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK F48 G49 Q54 L59 M63 T66 E67 S68 E69 N70 G71 T72 I73 L79 F82 F83 I88 S92 I95 PHE ALA ALA HIS
TYR HIS HIS GLY ASP HIS MET ASP GLY ASN PRO PRO GLY GLY GLY ALA GLU HIS SER GLU HIS SER GLY HIS ASN GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	110.89Å 158.07Å 147.01Å 90.00° 107.47° 90.00°	Depositor
Resolution (Å)	50.06 – 3.60 50.06 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.06-3.60) 99.4 (50.06-3.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.14_3235, PHENIX 1.14_3235	Depositor
R, R_{free}	0.321 , 0.350 0.313 , 0.351	Depositor DCC
R_{free} test set	1723 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å^2)	109.7	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 57.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	17944	wwPDB-VP
Average B, all atoms (Å^2)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MQ7, HEA, CU

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	0.10	0/5022	0.31	0/6827
1	E	0.10	0/5022	0.30	0/6827
2	B	0.17	0/2122	0.44	0/2879
2	F	0.13	0/2122	0.40	0/2879
3	C	0.08	0/1452	0.25	0/1974
3	G	0.12	0/1452	0.32	0/1974
4	D	0.08	0/381	0.26	0/514
4	H	0.08	0/381	0.25	0/514
All	All	0.11	0/17954	0.33	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	140	0
1	E	4855	0	4855	146	0
2	B	2073	0	2061	68	0
2	F	2073	0	2061	74	0
3	C	1411	0	1444	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1411	0	1444	27	0
4	D	482	0	395	10	0
4	H	482	0	395	10	0
5	A	120	0	107	13	0
5	E	120	0	107	12	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
7	A	30	0	33	1	0
7	E	30	0	33	1	0
All	All	17944	0	17790	466	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (466) 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:E:170:MET:HG2	1:E:260:PHE:HB2	1.61	0.82
1:A:170:MET:HG2	1:A:260:PHE:HB2	1.63	0.79
1:E:349:MET:HE1	1:E:395:VAL:HG23	1.64	0.77
2:B:261:GLU:O	2:B:265:ARG:NH2	2.18	0.77
1:A:349:MET:HE1	1:A:395:VAL:HG23	1.66	0.76
1:A:39:LYS:HE3	1:A:43:LEU:HB2	1.69	0.75
1:E:409:THR:HA	1:E:476:PRO:HA	1.69	0.74
2:B:230:GLU:O	2:B:284:LYS:NZ	2.21	0.74
1:E:39:LYS:HE3	1:E:43:LEU:HB2	1.68	0.74
2:F:261:GLU:O	2:F:265:ARG:NH2	2.21	0.74
1:E:409:THR:O	1:E:411:PHE:N	2.20	0.73
1:E:108:ILE:HG21	1:E:190:LEU:HD22	1.71	0.72
2:F:229:ASP:OD2	2:F:265:ARG:NH1	2.22	0.72
1:E:326:VAL:O	1:E:329:HIS:ND1	2.22	0.72
1:A:409:THR:O	1:A:411:PHE:N	2.22	0.72
2:F:230:GLU:O	2:F:284:LYS:NZ	2.23	0.71
1:A:267:MET:HG2	3:C:51:ARG:HE	1.52	0.71
2:B:217:GLN:HA	2:B:243:SER:HB2	1.72	0.71
1:A:599:ALA:HB2	1:A:617:GLY:HA3	1.71	0.71
1:A:108:ILE:HG21	1:A:190:LEU:HD22	1.73	0.71
2:F:76:ILE:HA	2:F:79:VAL:HG22	1.73	0.70
1:A:409:THR:HA	1:A:476:PRO:HA	1.73	0.70
1:A:54:LYS:NZ	1:A:545:PRO:O	2.25	0.69
1:A:177:MET:HG2	1:A:179:PRO:HD2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:MET:HG2	1:E:179:PRO:HD2	1.75	0.68
2:B:229:ASP:OD2	2:B:265:ARG:NH1	2.27	0.67
2:B:268:TYR:HD1	2:B:279:PRO:HD2	1.59	0.67
2:B:221:PRO:O	2:B:243:SER:OG	2.11	0.66
1:A:445:ASN:HB3	1:A:448:ILE:HD11	1.76	0.66
3:C:85:VAL:HA	3:C:89:ARG:HB2	1.75	0.66
1:E:445:ASN:HB3	1:E:448:ILE:HD11	1.77	0.66
1:E:599:ALA:HB2	1:E:617:GLY:HA3	1.76	0.66
1:E:92:SER:O	1:E:96:ASN:ND2	2.29	0.66
1:E:54:LYS:NZ	1:E:545:PRO:O	2.29	0.65
1:A:92:SER:O	1:A:96:ASN:ND2	2.28	0.65
1:E:95:TYR:OH	5:E:1001:HEA:O1A	2.15	0.65
2:F:221:PRO:O	2:F:243:SER:OG	2.14	0.65
2:B:278:ASP:O	2:B:280:PHE:N	2.29	0.65
1:A:173:ALA:O	1:A:253:ARG:NH1	2.31	0.64
2:F:148:ASP:OD2	2:F:263:ARG:NH2	2.30	0.64
1:E:554:GLU:HB3	1:E:556:LYS:HE3	1.80	0.63
2:F:284:LYS:HD3	2:F:285:LYS:H	1.63	0.63
1:A:79:ARG:NH2	1:A:467:GLN:OE1	2.27	0.63
2:B:114:ASP:HB3	2:B:234:PRO:HB3	1.79	0.63
2:B:37:VAL:HG13	2:B:41:ILE:HD12	1.79	0.62
2:B:233:LEU:HD11	2:B:266:LEU:HD12	1.80	0.62
2:F:116:LYS:HD3	2:F:237:VAL:HG11	1.81	0.62
1:E:121:VAL:HG13	1:E:438:LYS:HZ3	1.64	0.62
1:A:326:VAL:HG22	1:A:329:HIS:HD2	1.63	0.62
3:C:186:ASP:HA	3:C:189:TRP:HB2	1.81	0.62
1:E:187:LEU:HD21	1:E:249:LEU:HG	1.81	0.62
1:A:82:LEU:O	1:A:492:ASN:ND2	2.33	0.62
1:E:82:LEU:O	1:E:492:ASN:ND2	2.32	0.62
1:A:187:LEU:HD21	1:A:249:LEU:HG	1.82	0.62
3:G:40:THR:HG23	1:E:274:LEU:HD22	1.82	0.61
1:E:173:ALA:O	1:E:253:ARG:NH1	2.33	0.61
1:A:49:THR:OG1	1:A:586:SER:O	2.19	0.61
1:A:121:VAL:HG13	1:A:438:LYS:HZ3	1.66	0.61
1:A:134:PHE:HZ	3:C:26:GLY:HA3	1.65	0.61
1:E:437:PRO:HG3	1:E:443:LYS:HB3	1.82	0.61
2:F:75:PRO:HB2	1:E:353:ILE:HD12	1.83	0.60
1:A:353:ILE:HD12	2:B:75:PRO:HB2	1.84	0.59
2:F:84:VAL:H	2:F:85:PRO:HD2	1.66	0.59
1:E:420:LEU:HD13	5:E:1002:HEA:HBC2	1.84	0.59
3:C:83:ILE:HD13	3:C:176:PHE:HD1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:163:TYR:HB2	1:E:334:MET:HA	1.84	0.59
1:A:334:MET:HA	2:B:163:TYR:HB2	1.83	0.59
1:A:378:LEU:HD23	1:A:381:LEU:HD12	1.83	0.59
1:A:437:PRO:HG3	1:A:443:LYS:HB3	1.83	0.59
2:B:43:LEU:O	2:B:45:LYS:N	2.35	0.59
1:A:337:SER:O	1:A:339:SER:N	2.34	0.59
2:B:84:VAL:H	2:B:85:PRO:HD2	1.67	0.59
1:E:66:ILE:HG23	7:E:1004:MQ7:H151	1.85	0.59
3:G:186:ASP:HA	3:G:189:TRP:HB2	1.85	0.58
1:A:607:TRP:HD1	1:A:611:GLY:HA2	1.68	0.58
1:E:79:ARG:NH2	1:E:467:GLN:OE1	2.32	0.58
1:E:286:VAL:O	1:E:424:THR:OG1	2.21	0.58
1:A:180:GLY:O	1:A:253:ARG:NH2	2.36	0.58
1:A:274:LEU:HD22	3:C:40:THR:HG23	1.86	0.58
1:A:344:PHE:O	1:A:348:THR:OG1	2.19	0.58
2:B:148:ASP:OD2	2:B:263:ARG:NH2	2.33	0.58
1:E:378:LEU:HD23	1:E:381:LEU:HD12	1.84	0.58
1:A:103:GLY:HA3	5:A:1001:HEA:HBD2	1.85	0.58
1:A:346:ILE:HD11	2:B:87:VAL:HG21	1.85	0.58
2:F:135:PRO:HG2	2:F:138:ARG:HD2	1.85	0.58
1:A:554:GLU:HB3	1:A:556:LYS:HE3	1.85	0.58
2:B:97:PRO:HG2	2:B:173:TYR:HB2	1.86	0.58
1:E:337:SER:O	1:E:339:SER:N	2.37	0.57
3:C:75:LEU:HD11	3:C:182:TRP:HE1	1.69	0.57
1:E:106:MET:O	1:E:108:ILE:N	2.34	0.57
1:A:412:LEU:HD13	5:A:1002:HEA:HBA1	1.85	0.57
1:A:412:LEU:HD11	5:A:1002:HEA:HAD2	1.85	0.57
2:B:175:GLN:NE2	2:B:176:ALA:O	2.38	0.57
1:E:315:SER:OG	1:E:354:PRO:O	2.22	0.57
1:A:414:SER:OG	1:A:464:PHE:O	2.19	0.57
2:F:267:GLY:HA3	2:F:281:GLU:HG3	1.85	0.57
1:A:66:ILE:HG23	7:A:1004:MQ7:H151	1.87	0.56
1:A:416:PHE:HZ	5:A:1001:HEA:HHD	1.70	0.56
2:F:278:ASP:O	2:F:280:PHE:N	2.38	0.56
1:E:607:TRP:HD1	1:E:611:GLY:HA2	1.70	0.56
1:A:48:ILE:HA	1:A:143:TRP:HZ2	1.71	0.56
2:F:214:LYS:O	2:F:214:LYS:HE2	2.05	0.56
1:E:123:VAL:HG13	1:E:225:THR:HG23	1.87	0.56
1:A:412:LEU:CD1	5:A:1002:HEA:HHA	2.35	0.56
3:C:75:LEU:HD21	3:C:182:TRP:HE1	1.70	0.56
2:F:165:MET:HE1	1:E:269:MET:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:412:LEU:HD11	5:E:1002:HEA:HAD2	1.86	0.56
1:E:126:GLN:HA	1:E:535:LEU:HB2	1.87	0.56
1:E:416:PHE:CZ	5:E:1001:HEA:HHD	2.40	0.56
1:E:470:LEU:HD11	1:E:492:ASN:HA	1.88	0.56
1:A:588:ARG:HE	1:A:624:LEU:HB3	1.71	0.55
2:B:76:ILE:HA	2:B:79:VAL:HG22	1.88	0.55
1:A:420:LEU:HD13	5:A:1002:HEA:HBC2	1.87	0.55
1:A:467:GLN:HA	1:A:470:LEU:HB2	1.88	0.55
2:B:135:PRO:HG2	2:B:138:ARG:HD2	1.88	0.55
2:F:154:TRP:HA	2:F:161:GLN:HB3	1.87	0.55
1:E:48:ILE:HA	1:E:143:TRP:HZ2	1.71	0.55
3:C:73:LEU:HD12	3:C:76:ILE:HD11	1.89	0.55
1:E:56:LEU:HD21	1:E:139:ASN:HA	1.89	0.55
1:E:555:VAL:HG13	1:E:560:ALA:HB2	1.89	0.55
1:E:467:GLN:HA	1:E:470:LEU:HB2	1.89	0.55
1:A:96:ASN:OD1	2:B:190:THR:OG1	2.16	0.54
1:A:331:PHE:O	1:A:333:THR:N	2.36	0.54
3:G:85:VAL:HA	3:G:89:ARG:HB2	1.87	0.54
1:A:96:ASN:HB3	1:A:163:ASN:HB2	1.89	0.54
3:G:26:GLY:HA3	1:E:134:PHE:HZ	1.73	0.54
4:D:50:PHE:O	4:D:54:GLN:NE2	2.39	0.54
1:E:408:ASN:HB3	1:E:477:ARG:HG2	1.88	0.54
1:E:412:LEU:HD13	5:E:1002:HEA:HBA1	1.90	0.54
1:A:106:MET:O	1:A:108:ILE:N	2.36	0.54
1:E:49:THR:OG1	1:E:586:SER:O	2.24	0.54
1:E:416:PHE:HZ	5:E:1001:HEA:HHD	1.71	0.54
1:A:349:MET:HE3	1:A:398:ALA:HB3	1.90	0.54
1:A:416:PHE:CZ	5:A:1001:HEA:HHD	2.42	0.54
1:A:319:ILE:HG23	1:A:354:PRO:HB2	1.90	0.53
2:B:100:THR:O	2:B:101:LYS:HG3	2.08	0.53
1:E:344:PHE:O	1:E:348:THR:OG1	2.19	0.53
1:E:414:SER:OG	1:E:464:PHE:O	2.21	0.53
1:A:57:GLY:HA3	1:A:121:VAL:HG23	1.90	0.53
1:A:204:PHE:HB2	1:A:232:MET:HG3	1.88	0.53
2:B:284:LYS:HD3	2:B:285:LYS:H	1.72	0.53
2:F:37:VAL:HG13	2:F:41:ILE:HD12	1.91	0.53
1:E:180:GLY:O	1:E:253:ARG:NH2	2.41	0.53
4:D:71:GLY:O	4:D:73:ILE:N	2.40	0.53
4:H:88:ILE:HG12	1:E:277:ILE:HD13	1.90	0.53
2:B:233:LEU:HB2	2:B:284:LYS:HZ1	1.74	0.53
1:E:140:LEU:HB3	1:E:589:PRO:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:158:ILE:HD12	3:C:175:ILE:HG13	1.90	0.53
1:A:123:VAL:HG13	1:A:225:THR:HG23	1.90	0.53
1:A:95:TYR:OH	5:A:1001:HEA:O1A	2.25	0.52
1:A:140:LEU:HB3	1:A:589:PRO:HB3	1.91	0.52
1:E:412:LEU:CD1	5:E:1002:HEA:HHA	2.40	0.52
2:B:269:GLN:NE2	2:F:281:GLU:OE2	2.43	0.52
4:H:71:GLY:O	4:H:73:ILE:N	2.40	0.52
2:F:233:LEU:HB2	2:F:284:LYS:HZ1	1.75	0.52
1:E:349:MET:HE3	1:E:398:ALA:HB3	1.91	0.52
2:F:102:ASP:OD1	2:F:102:ASP:N	2.40	0.52
1:E:242:LEU:HB2	1:E:278:TRP:CD1	2.44	0.52
1:A:242:LEU:HB2	1:A:278:TRP:CD1	2.45	0.52
1:A:315:SER:OG	1:A:354:PRO:O	2.28	0.52
1:A:115:LEU:HG	1:A:289:PRO:HB2	1.92	0.52
1:E:280:HIS:HA	1:E:283:VAL:HB	1.92	0.51
3:G:75:LEU:HD21	3:G:182:TRP:HE1	1.74	0.51
1:E:96:ASN:HB3	1:E:163:ASN:HB2	1.92	0.51
1:E:284:TYR:HA	1:E:287:ILE:HG22	1.92	0.51
1:A:286:VAL:O	1:A:424:THR:OG1	2.28	0.51
2:B:250:VAL:C	2:B:252:HIS:H	2.18	0.51
1:A:53:HIS:CD2	1:A:131:ASP:HA	2.46	0.51
1:E:166:TRP:H	5:E:1001:HEA:CGD	2.24	0.51
2:F:268:TYR:CD1	2:F:279:PRO:HD2	2.46	0.51
1:E:322:LEU:HB3	1:E:351:ILE:HD12	1.93	0.51
3:G:153:PHE:HA	3:G:156:THR:HG22	1.92	0.51
2:F:79:VAL:O	2:F:83:SER:N	2.44	0.51
3:C:122:VAL:HA	3:C:126:ALA:HB2	1.92	0.50
3:C:141:LEU:HA	3:C:144:HIS:HB3	1.92	0.50
3:G:93:LEU:HD23	3:G:93:LEU:H	1.76	0.50
1:E:47:TRP:O	1:E:49:THR:N	2.45	0.50
1:E:230:ILE:HG13	1:E:316:ILE:HG23	1.93	0.50
2:F:124:GLN:O	2:F:126:ILE:N	2.44	0.50
2:B:100:THR:HG21	2:B:139:PRO:HG3	1.94	0.50
2:B:106:LEU:HD22	2:B:138:ARG:HH21	1.76	0.50
2:F:250:VAL:C	2:F:252:HIS:H	2.20	0.50
1:E:301:PHE:HD2	1:E:377:MET:HG2	1.76	0.50
2:B:111:THR:HG21	2:B:252:HIS:CD2	2.47	0.50
2:F:240:LEU:HD12	2:F:242:PHE:HE1	1.76	0.50
1:E:115:LEU:HG	1:E:289:PRO:HB2	1.92	0.50
3:G:194:THR:HG21	4:H:54:GLN:HG3	1.92	0.50
2:B:185:ARG:NH1	2:B:195:ALA:O	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:LEU:HB2	2:B:284:LYS:NZ	2.27	0.50
1:A:53:HIS:HD2	1:A:131:ASP:HA	1.77	0.49
3:C:93:LEU:HD23	3:C:93:LEU:H	1.76	0.49
1:E:204:PHE:HB2	1:E:232:MET:HG3	1.94	0.49
1:E:588:ARG:HE	1:E:624:LEU:HB3	1.76	0.49
1:A:393:THR:HG21	1:A:468:TYR:CZ	2.46	0.49
2:F:29:LEU:HD21	5:E:1002:HEA:H243	1.94	0.49
2:F:120:SER:HA	2:F:127:GLU:HA	1.94	0.49
1:A:54:LYS:HZ3	1:A:544:PRO:HB2	1.78	0.49
2:B:120:SER:HB2	2:B:245:THR:HG23	1.93	0.49
2:B:240:LEU:HD12	2:B:242:PHE:HE1	1.75	0.49
3:G:26:GLY:HA3	1:E:134:PHE:CZ	2.47	0.49
1:A:555:VAL:HG13	1:A:560:ALA:HB2	1.94	0.49
1:A:470:LEU:HD11	1:A:492:ASN:HA	1.93	0.49
2:F:142:PHE:HB3	2:F:144:ILE:HD11	1.95	0.49
1:A:547:TYR:HA	1:A:581:HIS:HE2	1.77	0.49
1:A:392:VAL:HB	2:B:29:LEU:HB3	1.93	0.49
2:F:111:THR:HG21	2:F:252:HIS:CD2	2.48	0.49
1:A:47:TRP:O	1:A:49:THR:N	2.45	0.48
1:A:408:ASN:HB3	1:A:477:ARG:HG2	1.95	0.48
1:A:54:LYS:NZ	1:A:544:PRO:HB2	2.28	0.48
1:A:134:PHE:CZ	3:C:26:GLY:HA3	2.44	0.48
1:A:284:TYR:HA	1:A:287:ILE:HG22	1.94	0.48
2:F:113:VAL:HA	2:F:147:ALA:HB3	1.95	0.48
3:C:22:LEU:HD23	3:C:22:LEU:H	1.78	0.48
1:E:220:ARG:HB3	1:E:558:GLN:HG3	1.94	0.48
2:B:124:GLN:O	2:B:126:ILE:N	2.47	0.48
1:E:319:ILE:HG23	1:E:354:PRO:HB2	1.95	0.48
1:E:376:PRO:HB3	1:E:434:PHE:HB2	1.96	0.48
3:C:194:THR:HG21	4:D:54:GLN:HG3	1.96	0.48
1:E:623:VAL:O	1:E:626:SER:OG	2.32	0.48
1:A:623:VAL:O	1:A:626:SER:OG	2.30	0.48
1:E:607:TRP:CD1	1:E:611:GLY:HA2	2.48	0.48
1:A:184:ASN:HB3	1:A:604:VAL:HG22	1.96	0.48
1:E:420:LEU:HD13	5:E:1002:HEA:CBC	2.43	0.48
1:A:301:PHE:HD2	1:A:377:MET:HG2	1.79	0.47
1:A:607:TRP:CD1	1:A:611:GLY:HA2	2.48	0.47
3:G:72:PHE:HA	3:G:75:LEU:HB3	1.96	0.47
1:E:280:HIS:CG	1:E:329:HIS:HE1	2.32	0.47
1:A:533:ARG:NH1	1:A:559:ASP:OD2	2.48	0.47
2:F:69:VAL:O	2:F:72:THR:OG1	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:100:THR:O	2:F:101:LYS:HG3	2.13	0.47
2:F:155:ILE:HA	2:F:184:GLY:HA2	1.96	0.47
2:F:185:ARG:NH1	2:F:195:ALA:O	2.40	0.47
1:E:133:ALA:HA	1:E:211:MET:HE1	1.96	0.47
2:B:101:LYS:HD3	2:B:102:ASP:H	1.79	0.47
1:A:21:VAL:HB	1:A:157:VAL:HG21	1.97	0.47
1:A:396:MET:O	1:A:406:TYR:OH	2.20	0.47
1:A:420:LEU:HD13	5:A:1002:HEA:CBC	2.44	0.47
2:F:233:LEU:HB2	2:F:284:LYS:NZ	2.30	0.47
1:E:326:VAL:HG22	1:E:329:HIS:HD1	1.78	0.47
1:E:547:TYR:HA	1:E:581:HIS:HE2	1.80	0.47
2:B:144:ILE:HD12	2:B:153:LEU:HD21	1.96	0.47
3:C:75:LEU:HD11	3:C:182:TRP:NE1	2.30	0.47
2:F:49:ARG:HE	1:E:370:ARG:HD3	1.79	0.47
2:F:233:LEU:HD11	2:F:266:LEU:HD12	1.97	0.47
1:E:373:PHE:CD1	1:E:381:LEU:HD11	2.49	0.47
4:D:67:GLU:HA	4:D:68:SER:HA	1.70	0.47
3:G:28:TRP:HZ2	4:H:66:THR:HG22	1.80	0.47
1:E:21:VAL:HB	1:E:157:VAL:HG21	1.97	0.47
1:A:412:LEU:HD11	5:A:1002:HEA:HHA	1.96	0.47
3:C:73:LEU:HD23	4:D:10:UNK:HA	1.97	0.47
3:G:155:ILE:O	3:G:159:LEU:HD23	2.15	0.47
3:G:188:VAL:HA	3:G:191:PHE:HB2	1.96	0.47
3:G:21:ARG:HA	3:G:21:ARG:HD3	1.80	0.46
2:F:43:LEU:O	2:F:45:LYS:N	2.45	0.46
2:F:36:PHE:O	2:F:40:THR:OG1	2.22	0.46
2:F:117:TRP:NE1	2:F:197:GLN:OE1	2.49	0.46
1:E:59:MET:HA	1:E:62:ILE:HG22	1.97	0.46
1:E:410:TYR:O	1:E:414:SER:N	2.37	0.46
3:C:61:LEU:HD12	3:C:64:VAL:HG23	1.97	0.46
1:E:134:PHE:O	1:E:203:ASN:ND2	2.49	0.46
1:E:298:ILE:HD12	1:E:377:MET:HE1	1.98	0.46
1:A:178:SER:HB2	2:B:270:ALA:O	2.16	0.46
1:A:206:VAL:HG21	3:C:26:GLY:HA2	1.97	0.46
2:B:158:LEU:HD13	2:B:174:LEU:HG	1.98	0.46
2:F:154:TRP:CD1	2:F:161:GLN:HE21	2.33	0.46
1:A:183:GLU:HG3	1:A:187:LEU:HD13	1.96	0.46
4:H:59:LEU:O	4:H:63:MET:HB2	2.16	0.46
4:H:68:SER:O	4:H:70:ASN:N	2.48	0.46
3:G:159:LEU:O	3:G:163:LYS:NZ	2.49	0.46
2:F:276:LYS:HD2	2:F:278:ASP:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:SER:OG	1:A:179:PRO:HD3	2.16	0.46
1:A:418:TYR:HA	1:A:460:PHE:HZ	1.80	0.46
2:B:142:PHE:HB3	2:B:144:ILE:HD11	1.98	0.46
3:C:24:ILE:O	3:C:28:TRP:HB2	2.16	0.45
1:A:373:PHE:CD1	1:A:381:LEU:HD11	2.51	0.45
3:C:188:VAL:HG23	3:C:189:TRP:HE3	1.80	0.45
2:F:29:LEU:HD22	1:E:395:VAL:HG11	1.96	0.45
1:E:235:ILE:O	1:E:239:PHE:HB2	2.16	0.45
1:E:353:ILE:HB	1:E:354:PRO:HD3	1.98	0.45
1:A:444:LEU:HG	1:A:512:ASN:HB3	1.98	0.45
2:F:268:TYR:HD1	2:F:279:PRO:HD2	1.79	0.45
1:E:183:GLU:HG3	1:E:187:LEU:HD13	1.99	0.45
1:E:105:ILE:HG22	1:E:106:MET:SD	2.57	0.45
1:E:296:GLU:O	1:E:300:SER:N	2.50	0.45
1:E:359:ILE:HA	1:E:362:TRP:CE3	2.51	0.45
1:E:428:CYS:O	1:E:432:PHE:HB2	2.16	0.45
1:E:533:ARG:NH1	1:E:559:ASP:OD2	2.49	0.45
1:A:280:HIS:HA	1:A:283:VAL:HB	1.98	0.45
1:A:326:VAL:HG22	1:A:329:HIS:CD2	2.48	0.45
1:A:588:ARG:NE	1:A:624:LEU:HB3	2.30	0.45
3:G:141:LEU:HA	3:G:144:HIS:HB3	1.98	0.45
1:A:230:ILE:HG13	1:A:316:ILE:HG23	1.99	0.45
1:A:353:ILE:HB	1:A:354:PRO:HD3	1.98	0.45
1:A:376:PRO:HB3	1:A:434:PHE:HB2	1.99	0.45
2:B:154:TRP:CD1	2:B:161:GLN:HE21	2.35	0.45
3:C:73:LEU:HD11	4:D:57:LEU:HD21	1.99	0.45
3:C:161:GLN:O	3:C:166:GLY:N	2.41	0.45
1:E:418:TYR:HA	1:E:460:PHE:HZ	1.81	0.45
1:A:39:LYS:HD2	1:A:39:LYS:HA	1.75	0.45
3:G:79:PHE:CD1	3:G:103:THR:HG21	2.51	0.45
4:H:68:SER:OG	4:H:69:GLU:N	2.50	0.45
1:E:54:LYS:NZ	1:E:544:PRO:HB2	2.32	0.45
1:E:349:MET:HA	1:E:349:MET:HE2	1.99	0.45
1:E:103:GLY:HA3	5:E:1001:HEA:HBD2	1.98	0.45
2:B:155:ILE:HA	2:B:184:GLY:HA2	1.98	0.45
1:A:127:ILE:HG13	1:A:129:ALA:H	1.82	0.44
4:D:59:LEU:O	4:D:63:MET:HB2	2.17	0.44
1:E:39:LYS:HD2	1:E:39:LYS:HA	1.74	0.44
1:E:208:ILE:HD13	1:E:229:LEU:HB2	1.99	0.44
1:A:105:ILE:HG22	1:A:106:MET:SD	2.58	0.44
1:A:337:SER:HB3	1:A:340:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:86:HIS:HD2	3:G:92:SER:HB2	1.82	0.44
2:F:144:ILE:HD12	2:F:153:LEU:HD21	1.99	0.44
1:A:54:LYS:NZ	1:A:548:ASN:HB3	2.31	0.44
1:A:235:ILE:O	1:A:239:PHE:HB2	2.17	0.44
1:A:349:MET:HE2	1:A:349:MET:HA	1.98	0.44
1:E:331:PHE:O	1:E:333:THR:N	2.41	0.44
1:A:273:ASN:HA	1:A:331:PHE:HZ	1.83	0.44
1:A:428:CYS:O	1:A:432:PHE:HB2	2.17	0.44
1:A:126:GLN:HA	1:A:535:LEU:HB2	1.99	0.44
3:C:190:ILE:HG21	4:D:57:LEU:HD13	1.99	0.44
3:G:86:HIS:CD2	3:G:92:SER:HB2	2.53	0.44
2:F:87:VAL:HG21	1:E:346:ILE:HD11	1.99	0.44
2:B:214:LYS:HB3	2:B:214:LYS:HE3	1.76	0.44
2:F:178:LYS:O	2:F:182:TYR:OH	2.21	0.44
1:E:178:SER:OG	1:E:179:PRO:HD3	2.18	0.44
1:E:184:ASN:HB3	1:E:604:VAL:HG22	1.98	0.44
2:B:250:VAL:O	2:B:252:HIS:N	2.41	0.44
2:B:163:TYR:CZ	2:B:189:PHE:HZ	2.36	0.44
3:G:104:LEU:HD11	3:G:152:ILE:HG23	1.99	0.43
4:H:70:ASN:OD1	1:E:210:LYS:NZ	2.51	0.43
1:E:127:ILE:HG13	1:E:129:ALA:H	1.83	0.43
2:B:245:THR:HG22	2:B:247:LEU:H	1.83	0.43
2:F:27:PHE:HA	2:F:30:PHE:HB2	2.00	0.43
1:E:187:LEU:HD23	1:E:250:SER:HA	2.00	0.43
1:A:121:VAL:HG13	1:A:438:LYS:NZ	2.32	0.43
3:C:72:PHE:HA	3:C:75:LEU:HB3	2.00	0.43
1:E:133:ALA:N	1:E:207:THR:OG1	2.47	0.43
1:A:56:LEU:HA	1:A:59:MET:HE2	2.00	0.43
1:A:110:MET:O	1:A:114:PHE:HB2	2.19	0.43
1:A:221:MET:N	1:A:222:PRO:HA	2.34	0.43
1:A:599:ALA:HA	1:A:614:GLY:HA2	2.00	0.43
2:B:114:ASP:C	2:B:116:LYS:H	2.27	0.43
3:C:188:VAL:HA	3:C:191:PHE:HB2	2.00	0.43
1:E:280:HIS:ND1	1:E:329:HIS:HE1	2.16	0.43
1:E:326:VAL:HG22	1:E:329:HIS:ND1	2.34	0.43
1:A:68:LEU:HD22	5:A:1001:HEA:H262	1.99	0.43
1:A:231:THR:HG23	1:A:285:ILE:HG23	2.00	0.43
3:G:167:LEU:HB3	3:G:172:SER:HB2	2.01	0.43
2:F:163:TYR:OH	1:E:407:HIS:NE2	2.46	0.43
1:A:41:LYS:HD2	1:A:41:LYS:HA	1.85	0.43
2:B:146:SER:OG	2:B:149:SER:O	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:114:ASP:O	2:F:116:LYS:N	2.44	0.43
1:E:361:ASN:O	1:E:365:THR:OG1	2.23	0.43
2:B:101:LYS:CG	2:B:102:ASP:H	2.31	0.43
4:D:90:LEU:O	4:D:94:TRP:HB2	2.19	0.43
1:E:54:LYS:NZ	1:E:548:ASN:HB3	2.33	0.43
1:E:221:MET:N	1:E:222:PRO:HA	2.34	0.43
1:A:202:ILE:HG23	3:C:29:ILE:HD11	2.01	0.43
1:A:384:ILE:HB	1:A:385:PRO:HD3	2.00	0.43
2:B:144:ILE:HG22	2:B:164:ALA:HA	2.00	0.43
2:F:71:TRP:O	2:F:75:PRO:HD3	2.19	0.43
2:F:114:ASP:C	2:F:116:LYS:H	2.26	0.43
2:B:114:ASP:O	2:B:116:LYS:N	2.46	0.42
2:F:49:ARG:HG2	1:E:370:ARG:NE	2.34	0.42
2:F:250:VAL:O	2:F:252:HIS:N	2.44	0.42
1:E:185:TYR:CD1	1:E:604:VAL:HG11	2.54	0.42
1:E:367:TYR:C	1:E:369:GLY:H	2.27	0.42
1:A:367:TYR:C	1:A:369:GLY:H	2.26	0.42
1:E:393:THR:HG21	1:E:468:TYR:CZ	2.54	0.42
2:B:260:MET:O	2:B:264:LYS:HB2	2.20	0.42
1:A:187:LEU:HD23	1:A:250:SER:HA	2.01	0.42
1:A:551:VAL:HG22	1:A:572:TYR:HD1	1.84	0.42
4:H:67:GLU:HA	4:H:68:SER:HA	1.68	0.42
1:E:384:ILE:HB	1:E:385:PRO:HD3	2.00	0.42
1:E:313:VAL:O	1:E:316:ILE:HG22	2.20	0.42
1:A:476:PRO:HG3	2:B:154:TRP:HZ3	1.84	0.42
2:B:71:TRP:O	2:B:75:PRO:HD3	2.20	0.42
2:F:74:ILE:N	2:F:75:PRO:CD	2.83	0.42
2:B:154:TRP:HA	2:B:161:GLN:HB3	2.02	0.42
2:F:101:LYS:HE3	2:F:101:LYS:HB2	1.85	0.42
1:E:57:GLY:HA3	1:E:121:VAL:HG23	2.02	0.42
1:A:446:GLU:O	1:A:450:LYS:HD3	2.20	0.42
2:B:127:GLU:CD	2:B:246:HIS:HD2	2.27	0.42
2:F:106:LEU:HD23	2:F:140:ILE:HG22	2.02	0.42
1:E:100:THR:O	1:E:104:THR:OG1	2.37	0.42
1:E:530:GLY:HA3	1:E:537:TRP:HZ3	1.85	0.42
1:A:367:TYR:CZ	2:B:43:LEU:HB2	2.55	0.42
3:G:29:ILE:HD11	1:E:202:ILE:HG23	2.01	0.42
1:E:424:THR:O	1:E:428:CYS:N	2.42	0.42
1:A:140:LEU:O	1:A:144:THR:OG1	2.29	0.42
1:A:244:VAL:HA	1:A:247:ALA:HB3	2.01	0.42
3:G:25:LEU:HD12	1:E:206:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:28:TRP:CZ2	4:H:66:THR:HG22	2.54	0.42
1:E:170:MET:N	1:E:171:PRO:HD2	2.35	0.42
1:E:209:LEU:C	1:E:210:LYS:HD2	2.45	0.42
3:C:187:VAL:HA	4:D:58:GLN:CD	2.45	0.41
1:E:77:MET:HA	1:E:80:ALA:HB3	2.02	0.41
1:E:115:LEU:HD12	1:E:115:LEU:HA	1.91	0.41
1:E:120:ASN:HA	1:E:204:PHE:HZ	1.85	0.41
1:E:198:LEU:HD11	1:E:240:PRO:HG3	2.01	0.41
1:E:244:VAL:HA	1:E:247:ALA:HB3	2.01	0.41
1:A:170:MET:N	1:A:171:PRO:HD2	2.35	0.41
1:A:322:LEU:HB3	1:A:351:ILE:HD12	2.02	0.41
1:A:377:MET:O	1:A:381:LEU:N	2.50	0.41
1:A:586:SER:O	1:A:589:PRO:HD2	2.20	0.41
2:B:272:SER:OG	2:B:273:PRO:HD3	2.20	0.41
1:E:106:MET:HB3	1:E:107:ILE:HD12	2.01	0.41
1:E:240:PRO:O	1:E:244:VAL:HG22	2.21	0.41
1:E:267:MET:HB2	1:E:270:LEU:HB2	2.00	0.41
1:E:283:VAL:HG13	5:E:1002:HEA:C3C	2.49	0.41
1:A:99:PHE:CE2	1:A:478:ARG:HG2	2.55	0.41
2:B:27:PHE:HA	2:B:30:PHE:HB2	2.02	0.41
2:F:30:PHE:O	2:F:34:VAL:HG23	2.20	0.41
2:F:125:ASP:C	2:F:126:ILE:HG13	2.45	0.41
1:A:410:TYR:O	1:A:414:SER:N	2.40	0.41
2:B:287:GLU:HG2	2:B:288:PHE:H	1.86	0.41
2:F:74:ILE:N	2:F:75:PRO:HD3	2.35	0.41
1:E:106:MET:HA	1:E:110:MET:HB3	2.01	0.41
1:A:185:TYR:CD1	1:A:604:VAL:HG11	2.55	0.41
1:A:397:LEU:HD12	5:A:1002:HEA:HBA2	2.01	0.41
3:G:90:ARG:HH11	3:G:90:ARG:HA	1.86	0.41
2:F:228:TYR:HD2	2:F:249:TYR:HD2	1.67	0.41
2:F:276:LYS:HB3	2:F:277:THR:H	1.67	0.41
1:A:166:TRP:H	5:A:1001:HEA:CGD	2.33	0.41
2:B:107:VAL:O	2:B:122:PRO:HD2	2.20	0.41
2:B:264:LYS:O	2:F:264:LYS:HB3	2.19	0.41
2:B:276:LYS:HB3	2:B:277:THR:H	1.62	0.41
1:E:82:LEU:HD21	1:E:480:TYR:HA	2.03	0.41
1:E:588:ARG:NE	1:E:624:LEU:HB3	2.36	0.41
1:A:509:LEU:O	1:A:513:ILE:HG13	2.21	0.41
2:B:25:ILE:HA	2:B:25:ILE:HD12	1.84	0.41
2:F:163:TYR:CZ	2:F:189:PHE:HZ	2.38	0.41
2:F:276:LYS:HE2	2:F:277:THR:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:THR:CB	2:B:139:PRO:HG3	2.51	0.41
3:C:144:HIS:CE1	3:C:189:TRP:CE2	3.08	0.41
2:F:148:ASP:OD1	2:F:148:ASP:N	2.53	0.41
1:E:41:LYS:HA	1:E:41:LYS:HD2	1.87	0.41
1:A:106:MET:HA	1:A:110:MET:HB3	2.03	0.41
2:B:115:TRP:HD1	2:B:234:PRO:HA	1.86	0.41
3:C:188:VAL:HG23	3:C:189:TRP:CE3	2.54	0.41
3:G:87:GLU:HB3	3:G:169:PRO:HB3	2.02	0.41
3:G:193:PHE:HA	3:G:197:TYR:HD2	1.86	0.41
1:E:97:GLU:HB3	1:E:161:SER:HB2	2.01	0.41
1:A:424:THR:O	1:A:428:CYS:N	2.43	0.41
2:B:148:ASP:N	2:B:148:ASP:OD1	2.53	0.41
2:F:112:SER:O	2:F:147:ALA:N	2.49	0.41
2:F:284:LYS:CD	2:F:285:LYS:H	2.33	0.41
1:A:472:LEU:HD23	1:A:472:LEU:HA	1.94	0.40
1:A:50:THR:HA	1:A:585:ASN:ND2	2.36	0.40
1:E:242:LEU:HB2	1:E:278:TRP:CG	2.57	0.40
1:E:306:LEU:HD23	1:E:365:THR:HG21	2.03	0.40
2:B:278:ASP:O	2:B:279:PRO:C	2.65	0.40
2:F:67:LEU:O	2:F:70:VAL:HG12	2.21	0.40
2:F:163:TYR:CD2	1:E:334:MET:HB3	2.56	0.40
2:F:287:GLU:HG2	2:F:288:PHE:H	1.85	0.40
1:E:287:ILE:HD12	1:E:287:ILE:HA	1.95	0.40
1:A:198:LEU:HD11	1:A:240:PRO:HG3	2.04	0.40
1:A:448:ILE:H	1:A:448:ILE:HG13	1.67	0.40
3:C:55:GLY:C	2:F:225:LYS:HE3	2.47	0.40
2:F:227:LYS:O	2:F:231:LEU:HG	2.21	0.40
1:E:509:LEU:O	1:E:513:ILE:HG13	2.21	0.40
1:A:141:SER:OG	1:A:200:THR:OG1	2.37	0.40
1:A:208:ILE:HD13	1:A:229:LEU:HB2	2.02	0.40
1:A:240:PRO:O	1:A:244:VAL:HG22	2.22	0.40
1:E:141:SER:OG	1:E:200:THR:OG1	2.39	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%)	512 (85%)	76 (13%)	15 (2%)	4	28
1	E	603/655 (92%)	511 (85%)	75 (12%)	17 (3%)	4	26
2	B	250/296 (84%)	188 (75%)	51 (20%)	11 (4%)	2	18
2	F	250/296 (84%)	191 (76%)	48 (19%)	11 (4%)	2	18
3	C	176/204 (86%)	158 (90%)	17 (10%)	1 (1%)	21	54
3	G	176/204 (86%)	159 (90%)	16 (9%)	1 (1%)	21	54
4	D	46/124 (37%)	39 (85%)	6 (13%)	1 (2%)	5	30
4	H	46/124 (37%)	39 (85%)	6 (13%)	1 (2%)	5	30
All	All	2150/2558 (84%)	1797 (84%)	295 (14%)	58 (3%)	4	27

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	SER
1	A	222	PRO
1	A	239	PHE
1	A	548	ASN
2	B	279	PRO
2	F	125	ASP
2	F	279	PRO
1	E	178	SER
1	E	222	PRO
1	E	239	PHE
1	E	548	ASN
1	A	48	ILE
1	A	130	ARG
1	A	306	LEU
1	A	555	VAL
1	A	583	PRO
2	B	97	PRO
2	B	125	ASP
2	B	192	GLU
2	B	215	LYS
4	H	69	GLU
2	F	215	LYS
2	F	283	VAL

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Mol	Chain	Res	Type
1	E	48	ILE
1	E	130	ARG
1	E	306	LEU
1	E	410	TYR
1	E	555	VAL
1	E	583	PRO
1	A	221	MET
1	A	410	TYR
1	A	570	GLU
2	B	242	PHE
3	C	124	GLU
4	D	69	GLU
2	F	192	GLU
2	F	242	PHE
2	F	281	GLU
1	E	221	MET
1	E	570	GLU
1	A	338	ALA
2	B	84	VAL
2	B	273	PRO
2	B	281	GLU
2	F	273	PRO
1	E	338	ALA
1	A	41	LYS
1	A	549	PHE
2	B	283	VAL
3	G	124	GLU
2	F	84	VAL
1	E	41	LYS
1	E	86	ASN
2	F	240	LEU
1	E	549	PHE
2	F	96	ALA
2	B	278	ASP
1	E	474	GLY

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	512/558 (92%)	486 (95%)	26 (5%)	21	49
1	E	512/558 (92%)	488 (95%)	24 (5%)	23	50
2	B	230/263 (88%)	210 (91%)	20 (9%)	9	34
2	F	230/263 (88%)	203 (88%)	27 (12%)	5	25
3	C	151/171 (88%)	142 (94%)	9 (6%)	17	45
3	G	151/171 (88%)	141 (93%)	10 (7%)	15	43
4	D	38/59 (64%)	36 (95%)	2 (5%)	20	48
4	H	38/59 (64%)	36 (95%)	2 (5%)	20	48
All	All	1862/2102 (89%)	1742 (94%)	120 (6%)	16	43

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ARG
1	A	105	ILE
1	A	115	LEU
1	A	145	PHE
1	A	151	LEU
1	A	166	TRP
1	A	172	LEU
1	A	187	LEU
1	A	208	ILE
1	A	216	MET
1	A	239	PHE
1	A	260	PHE
1	A	273	ASN
1	A	283	VAL
1	A	328	THR
1	A	340	VAL
1	A	363	LEU
1	A	395	VAL
1	A	415	HIS
1	A	416	PHE
1	A	444	LEU
1	A	500	PHE
1	A	509	LEU
1	A	552	LEU
1	A	581	HIS

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Mol	Chain	Res	Type
1	A	633	TYR
2	B	20	LEU
2	B	29	LEU
2	B	39	PHE
2	B	101	LYS
2	B	115	TRP
2	B	128	THR
2	B	153	LEU
2	B	165	MET
2	B	174	LEU
2	B	175	GLN
2	B	188	ASN
2	B	213	VAL
2	B	217	GLN
2	B	223	LEU
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	59	ASP
3	C	61	LEU
3	C	75	LEU
3	C	85	VAL
3	C	97	VAL
3	C	128	LEU
3	C	144	HIS
4	D	69	GLU
4	D	79	LEU
3	G	25	LEU
3	G	56	VAL
3	G	59	ASP
3	G	61	LEU
3	G	75	LEU
3	G	85	VAL
3	G	97	VAL
3	G	128	LEU
3	G	161	GLN
3	G	192	ILE

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Mol	Chain	Res	Type
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	98	GLU
2	F	101	LYS
2	F	102	ASP
2	F	115	TRP
2	F	128	THR
2	F	153	LEU
2	F	165	MET
2	F	174	LEU
2	F	175	GLN
2	F	181	THR
2	F	188	ASN
2	F	217	GLN
2	F	223	LEU
2	F	224	THR
2	F	237	VAL
2	F	246	HIS
2	F	252	HIS
2	F	272	SER
2	F	276	LYS
2	F	277	THR
2	F	283	VAL
2	F	284	LYS
1	E	79	ARG
1	E	104	THR
1	E	105	ILE
1	E	115	LEU
1	E	145	PHE
1	E	151	LEU
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

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Mol	Chain	Res	Type
1	E	283	VAL
1	E	340	VAL
1	E	363	LEU
1	E	395	VAL
1	E	415	HIS
1	E	416	PHE
1	E	444	LEU
1	E	500	PHE
1	E	509	LEU
1	E	552	LEU
1	E	581	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	87	ASN
1	A	408	ASN
1	A	558	GLN
2	B	88	GLN
2	B	246	HIS
2	B	252	HIS
4	H	54	GLN
4	H	58	GLN
1	E	93	ASN
1	E	184	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	MQ7	A	1004	-	31,31,49	1.74	2 (6%)	38,41,63	1.44	8 (21%)
5	HEA	A	1001	1	66,67,67	2.55	27 (40%)	78,103,103	2.53	30 (38%)
5	HEA	A	1002	1	66,67,67	2.47	26 (39%)	78,103,103	2.73	33 (42%)
7	MQ7	E	1004	-	31,31,49	1.74	2 (6%)	38,41,63	1.47	8 (21%)
5	HEA	E	1001	1	66,67,67	2.54	26 (39%)	78,103,103	2.52	30 (38%)
5	HEA	E	1002	1	66,67,67	2.47	26 (39%)	78,103,103	2.71	33 (42%)

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	MQ7	A	1004	-	-	6/20/40/61	0/2/2/2
5	HEA	A	1001	1	-	13/36/76/76	-
5	HEA	A	1002	1	-	9/36/76/76	-
7	MQ7	E	1004	-	-	6/20/40/61	0/2/2/2
5	HEA	E	1001	1	-	13/36/76/76	-
5	HEA	E	1002	1	-	9/36/76/76	-

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1004	MQ7	C3-C2	7.82	1.49	1.35
7	E	1004	MQ7	C3-C2	7.81	1.49	1.35
5	A	1001	HEA	C3B-C2B	5.66	1.47	1.34
5	E	1001	HEA	C3B-C2B	5.64	1.47	1.34
5	E	1002	HEA	FE-ND	5.61	2.12	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	HEA	C3A-C2A	5.60	1.48	1.36
5	A	1002	HEA	FE-ND	5.59	2.12	1.94
5	E	1001	HEA	C3A-C2A	5.56	1.48	1.36
5	A	1002	HEA	FE-NB	5.55	2.12	1.94
5	E	1002	HEA	FE-NB	5.54	2.12	1.94
5	E	1002	HEA	C3B-C2B	5.54	1.47	1.34
5	A	1002	HEA	C3B-C2B	5.53	1.47	1.34
5	A	1001	HEA	FE-ND	5.32	2.11	1.94
5	E	1001	HEA	FE-ND	5.31	2.11	1.94
5	A	1002	HEA	C3A-C2A	5.27	1.48	1.36
5	E	1002	HEA	C3A-C2A	5.26	1.48	1.36
5	A	1001	HEA	C3D-C2D	5.22	1.47	1.36
5	E	1001	HEA	C3D-C2D	5.20	1.47	1.36
5	E	1001	HEA	FE-NB	5.13	2.10	1.94
5	A	1001	HEA	FE-NB	5.13	2.10	1.94
7	E	1004	MQ7	C10-C5	5.04	1.49	1.40
5	A	1002	HEA	C3D-C2D	5.02	1.47	1.36
5	E	1002	HEA	C3D-C2D	5.00	1.47	1.36
7	A	1004	MQ7	C10-C5	4.96	1.48	1.40
5	A	1002	HEA	FE-NC	4.83	2.11	1.95
5	E	1002	HEA	FE-NC	4.82	2.11	1.95
5	A	1001	HEA	CHB-C4A	4.71	1.47	1.38
5	A	1001	HEA	CHD-C1D	4.68	1.48	1.38
5	E	1001	HEA	CHB-C4A	4.68	1.47	1.38
5	A	1001	HEA	CHA-C1A	4.61	1.47	1.38
5	A	1001	HEA	CHC-C4B	4.60	1.47	1.38
5	E	1001	HEA	CHD-C1D	4.60	1.47	1.38
5	A	1001	HEA	FE-NC	4.59	2.10	1.95
5	E	1001	HEA	CHC-C4B	4.58	1.47	1.38
5	E	1001	HEA	FE-NC	4.57	2.10	1.95
5	E	1001	HEA	CHA-C1A	4.57	1.47	1.38
5	A	1002	HEA	CHB-C4A	4.33	1.46	1.38
5	E	1002	HEA	CHB-C4A	4.32	1.46	1.38
5	A	1002	HEA	CHC-C4B	4.32	1.47	1.38
5	A	1002	HEA	CHD-C1D	4.28	1.47	1.38
5	E	1002	HEA	CHD-C1D	4.26	1.47	1.38
5	E	1002	HEA	CHC-C4B	4.22	1.47	1.38
5	E	1002	HEA	CHA-C1A	4.19	1.46	1.38
5	A	1002	HEA	CHA-C1A	4.12	1.46	1.38
5	E	1002	HEA	C1A-NA	3.89	1.47	1.39
5	A	1002	HEA	C1A-NA	3.86	1.47	1.39
5	E	1001	HEA	CHC-C1C	3.82	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	HEA	CHC-C1C	3.74	1.47	1.39
5	E	1002	HEA	C4A-NA	3.73	1.47	1.39
5	A	1002	HEA	C4A-NA	3.73	1.47	1.39
5	A	1001	HEA	CHD-C4C	3.70	1.47	1.39
5	E	1001	HEA	C1A-NA	3.68	1.46	1.39
5	A	1001	HEA	C1A-NA	3.68	1.46	1.39
5	A	1001	HEA	CHB-C1B	3.66	1.47	1.39
5	E	1001	HEA	CHD-C4C	3.65	1.47	1.39
5	A	1001	HEA	C4A-NA	3.64	1.46	1.39
5	E	1001	HEA	C4A-NA	3.64	1.46	1.39
5	E	1001	HEA	CHB-C1B	3.62	1.47	1.39
5	E	1002	HEA	CHD-C4C	3.53	1.47	1.39
5	A	1002	HEA	CHD-C4C	3.52	1.47	1.39
5	A	1002	HEA	CHC-C1C	3.45	1.47	1.39
5	E	1002	HEA	CHC-C1C	3.42	1.47	1.39
5	A	1001	HEA	CHA-C4D	3.40	1.47	1.39
5	E	1001	HEA	CHA-C4D	3.34	1.46	1.39
5	E	1002	HEA	CHB-C1B	3.22	1.46	1.39
5	A	1002	HEA	CHB-C1B	3.20	1.46	1.39
5	E	1002	HEA	CHA-C4D	3.07	1.46	1.39
5	A	1002	HEA	CHA-C4D	3.03	1.46	1.39
5	E	1001	HEA	C1D-ND	-2.89	1.35	1.40
5	E	1001	HEA	C4B-NB	-2.81	1.35	1.40
5	E	1001	HEA	C4B-C3B	2.80	1.49	1.44
5	A	1001	HEA	C4B-NB	-2.79	1.35	1.40
5	A	1001	HEA	C1D-ND	-2.79	1.35	1.40
5	A	1001	HEA	C4B-C3B	2.77	1.49	1.44
5	E	1002	HEA	C4B-NB	-2.72	1.35	1.40
5	A	1002	HEA	C4B-C3B	2.71	1.49	1.44
5	A	1002	HEA	C4B-NB	-2.71	1.35	1.40
5	E	1002	HEA	C4B-C3B	2.69	1.49	1.44
5	E	1002	HEA	C1D-ND	-2.64	1.35	1.40
5	A	1002	HEA	C1D-ND	-2.63	1.35	1.40
5	A	1001	HEA	C1A-C2A	2.60	1.49	1.45
5	E	1001	HEA	C1A-C2A	2.59	1.49	1.45
5	E	1001	HEA	C1C-C2C	2.59	1.49	1.43
5	A	1001	HEA	C1C-C2C	2.54	1.49	1.43
5	A	1001	HEA	C3C-C4C	2.54	1.48	1.42
5	A	1001	HEA	C1D-C2D	2.49	1.49	1.44
5	E	1001	HEA	C3C-C4C	2.48	1.48	1.42
5	A	1002	HEA	C1C-C2C	2.46	1.49	1.43
5	E	1002	HEA	C1D-C2D	2.46	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1002	HEA	C1D-C2D	2.42	1.49	1.44
5	A	1002	HEA	C3C-C4C	2.42	1.48	1.42
5	E	1002	HEA	C1C-C2C	2.41	1.48	1.43
5	E	1002	HEA	C3C-C4C	2.41	1.48	1.42
5	E	1001	HEA	C1D-C2D	2.40	1.49	1.44
5	E	1001	HEA	C4C-NC	-2.36	1.35	1.39
5	E	1002	HEA	C4D-C3D	2.34	1.49	1.45
5	A	1002	HEA	C1A-C2A	2.31	1.49	1.45
5	E	1002	HEA	C1A-C2A	2.29	1.49	1.45
5	A	1001	HEA	C4C-NC	-2.25	1.35	1.39
5	A	1001	HEA	C4D-C3D	2.23	1.48	1.45
5	E	1001	HEA	C4D-C3D	2.22	1.48	1.45
5	A	1002	HEA	C4D-C3D	2.22	1.48	1.45
5	E	1002	HEA	C1B-C2B	2.16	1.48	1.44
5	A	1002	HEA	C1B-C2B	2.15	1.48	1.44
5	E	1002	HEA	C4C-NC	-2.13	1.35	1.39
5	A	1001	HEA	C1B-C2B	2.11	1.48	1.44
5	E	1001	HEA	C1B-C2B	2.09	1.48	1.44
5	A	1002	HEA	C4C-NC	-2.08	1.35	1.39
5	A	1001	HEA	C1C-NC	-2.00	1.35	1.39

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1002	HEA	C3D-C4D-ND	7.06	117.19	110.36
5	E	1002	HEA	C3D-C4D-ND	7.02	117.15	110.36
5	A	1002	HEA	C3C-C4C-NC	6.85	114.47	110.25
5	E	1002	HEA	C3C-C4C-NC	6.77	114.41	110.25
5	A	1001	HEA	C3D-C4D-ND	5.99	116.16	110.36
5	E	1001	HEA	C3D-C4D-ND	5.99	116.15	110.36
5	E	1001	HEA	C3C-C4C-NC	5.91	113.88	110.25
5	A	1001	HEA	C3C-C4C-NC	5.85	113.85	110.25
5	A	1002	HEA	C2B-C1B-NB	5.74	116.76	109.88
5	E	1002	HEA	C2B-C1B-NB	5.71	116.73	109.88
5	A	1002	HEA	C2A-C1A-NA	5.67	115.84	110.32
5	E	1002	HEA	C2A-C1A-NA	5.57	115.74	110.32
5	E	1002	HEA	C3C-C2C-C1C	-5.50	100.52	107.16
5	A	1001	HEA	CHA-C4D-ND	-5.47	118.47	124.42
5	E	1002	HEA	C3B-C4B-NB	5.45	116.30	109.84
5	A	1002	HEA	C3C-C2C-C1C	-5.45	100.58	107.16
5	A	1002	HEA	C2D-C1D-ND	5.44	116.29	109.84
5	E	1001	HEA	CHA-C4D-ND	-5.43	118.52	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1002	HEA	C2D-C1D-ND	5.40	116.24	109.84
5	A	1002	HEA	C3B-C4B-NB	5.37	116.20	109.84
5	A	1001	HEA	C3C-C2C-C1C	-5.22	100.87	107.16
5	E	1001	HEA	C3C-C2C-C1C	-5.22	100.87	107.16
5	A	1001	HEA	CHA-C1A-NA	-5.20	118.81	124.44
5	A	1002	HEA	C4A-NA-C1A	-5.08	100.37	105.35
5	E	1002	HEA	C4A-NA-C1A	-5.06	100.40	105.35
5	E	1001	HEA	CHA-C1A-NA	-4.99	119.04	124.44
5	A	1001	HEA	C2A-C1A-NA	4.90	115.09	110.32
5	E	1001	HEA	C2A-C1A-NA	4.84	115.03	110.32
5	E	1001	HEA	C2D-C1D-ND	4.65	115.35	109.84
5	E	1001	HEA	C2B-C1B-NB	4.59	115.38	109.88
5	A	1001	HEA	C3B-C4B-NB	4.58	115.27	109.84
5	E	1002	HEA	C2C-C1C-NC	4.58	117.05	110.08
5	A	1001	HEA	C2B-C1B-NB	4.56	115.34	109.88
5	A	1002	HEA	C2C-C1C-NC	4.53	116.97	110.08
5	A	1001	HEA	C2D-C1D-ND	4.53	115.20	109.84
5	E	1001	HEA	C3B-C4B-NB	4.50	115.17	109.84
5	E	1001	HEA	C1A-CHA-C4D	-4.48	116.40	126.06
5	A	1001	HEA	C1A-CHA-C4D	-4.35	116.67	126.06
5	A	1002	HEA	C3A-C2A-C1A	-4.23	103.03	107.08
5	A	1002	HEA	C1D-C2D-C3D	-4.20	102.55	106.96
5	E	1002	HEA	C3A-C2A-C1A	-4.12	103.14	107.08
5	E	1002	HEA	C1D-C2D-C3D	-4.10	102.64	106.96
5	A	1001	HEA	C3A-C2A-C1A	-4.08	103.18	107.08
5	E	1002	HEA	CHA-C4D-ND	-4.07	120.00	124.42
5	E	1001	HEA	C3A-C2A-C1A	-4.02	103.23	107.08
5	A	1002	HEA	CHA-C4D-ND	-4.01	120.06	124.42
5	A	1001	HEA	C2C-C1C-NC	4.00	116.16	110.08
5	A	1001	HEA	C4A-NA-C1A	-3.95	101.48	105.35
5	E	1001	HEA	C4A-NA-C1A	-3.93	101.50	105.35
5	E	1001	HEA	C1D-C2D-C3D	-3.93	102.82	106.96
5	A	1001	HEA	C1D-C2D-C3D	-3.92	102.84	106.96
5	E	1001	HEA	C2C-C1C-NC	3.89	116.00	110.08
5	A	1002	HEA	C1B-C2B-C3B	-3.85	102.19	106.80
5	E	1002	HEA	C1B-C2B-C3B	-3.80	102.25	106.80
5	A	1002	HEA	CHA-C1A-NA	-3.64	120.50	124.44
5	E	1002	HEA	C4D-C3D-C2D	-3.47	101.84	106.90
5	A	1002	HEA	C4D-C3D-C2D	-3.43	101.90	106.90
5	E	1002	HEA	CHA-C1A-NA	-3.42	120.74	124.44
5	E	1001	HEA	C4D-C3D-C2D	-3.27	102.13	106.90
7	A	1004	MQ7	C11-C12-C13	-3.24	121.40	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1001	HEA	C4D-C3D-C2D	-3.24	102.18	106.90
5	E	1001	HEA	C1B-C2B-C3B	-3.21	102.96	106.80
7	E	1004	MQ7	C11-C12-C13	-3.19	121.49	126.79
5	E	1002	HEA	C13-C14-C15	-3.18	120.00	127.66
5	A	1001	HEA	C1B-C2B-C3B	-3.17	103.01	106.80
5	A	1002	HEA	C13-C14-C15	-3.14	120.10	127.66
5	A	1002	HEA	C13-C12-C11	-3.05	109.76	114.35
5	E	1002	HEA	C26-C15-C16	3.02	120.35	115.27
5	A	1002	HEA	C26-C15-C16	3.02	120.35	115.27
5	E	1001	HEA	CHB-C1B-NB	-2.99	121.17	124.42
5	A	1001	HEA	C26-C15-C16	2.99	120.30	115.27
5	E	1002	HEA	CHB-C1B-NB	-2.98	121.18	124.42
5	A	1002	HEA	C27-C19-C20	2.98	120.28	115.27
7	E	1004	MQ7	C21-C22-C23	-2.97	120.52	127.66
5	A	1002	HEA	CHB-C1B-NB	-2.97	121.20	124.42
5	E	1001	HEA	C26-C15-C16	2.95	120.24	115.27
5	A	1001	HEA	CHB-C1B-NB	-2.94	121.23	124.42
7	E	1004	MQ7	C26-C25-C23	-2.93	109.82	114.62
5	A	1001	HEA	C4B-C3B-C2B	-2.91	102.43	107.41
5	A	1002	HEA	C1D-ND-C4D	-2.90	102.08	105.07
5	E	1002	HEA	C4B-C3B-C2B	-2.89	102.47	107.41
5	E	1001	HEA	C4B-C3B-C2B	-2.87	102.51	107.41
5	E	1002	HEA	C1D-ND-C4D	-2.86	102.12	105.07
7	A	1004	MQ7	C26-C25-C23	-2.86	109.94	114.62
7	A	1004	MQ7	C21-C22-C23	-2.86	120.78	127.66
5	A	1002	HEA	C4B-C3B-C2B	-2.84	102.56	107.41
5	E	1001	HEA	C17-C18-C19	-2.83	120.83	127.66
5	E	1002	HEA	C27-C19-C20	2.83	120.04	115.27
7	E	1004	MQ7	C14-C13-C15	2.83	120.03	115.27
5	A	1001	HEA	C27-C19-C20	2.78	119.95	115.27
5	A	1002	HEA	C17-C18-C19	-2.78	120.96	127.66
5	A	1001	HEA	C17-C18-C19	-2.74	121.05	127.66
7	A	1004	MQ7	C14-C13-C15	2.74	119.89	115.27
5	E	1002	HEA	C4B-NB-C1B	-2.73	102.25	105.07
5	E	1001	HEA	C27-C19-C20	2.71	119.84	115.27
5	A	1002	HEA	C4B-NB-C1B	-2.71	102.28	105.07
5	E	1002	HEA	C17-C18-C19	-2.69	121.18	127.66
7	E	1004	MQ7	C19-C18-C20	2.68	119.78	115.27
7	A	1004	MQ7	C16-C17-C18	-2.68	121.21	127.66
7	E	1004	MQ7	C24-C23-C25	2.63	119.70	115.27
5	E	1002	HEA	CHC-C1C-C2C	-2.63	119.81	127.24
7	E	1004	MQ7	C16-C17-C18	-2.62	121.34	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1002	HEA	CMB-C2B-C1B	2.62	129.03	125.04
5	A	1002	HEA	CHC-C1C-C2C	-2.59	119.94	127.24
5	A	1001	HEA	C13-C14-C15	-2.58	121.45	127.66
5	E	1002	HEA	C13-C12-C11	-2.56	110.50	114.35
7	A	1004	MQ7	C24-C23-C25	2.55	119.57	115.27
5	E	1002	HEA	CAD-C3D-C4D	2.55	129.11	124.66
5	E	1002	HEA	CMB-C2B-C1B	2.53	128.88	125.04
5	E	1001	HEA	C13-C14-C15	-2.52	121.59	127.66
7	A	1004	MQ7	C19-C18-C20	2.51	119.49	115.27
5	A	1002	HEA	C25-C23-C24	2.51	120.14	114.60
5	E	1001	HEA	CMB-C2B-C1B	2.50	128.85	125.04
5	A	1001	HEA	CMB-C2B-C1B	2.48	128.82	125.04
5	E	1001	HEA	CAD-C3D-C4D	2.46	128.96	124.66
5	A	1001	HEA	CHC-C4B-NB	-2.45	121.35	124.37
5	A	1001	HEA	C25-C23-C24	2.41	119.92	114.60
5	E	1001	HEA	CHC-C4B-NB	-2.41	121.41	124.37
5	E	1002	HEA	C25-C23-C24	2.40	119.91	114.60
5	A	1001	HEA	CMD-C2D-C1D	2.40	128.69	125.04
5	E	1001	HEA	C25-C23-C24	2.38	119.86	114.60
5	A	1002	HEA	CMD-C2D-C1D	2.38	128.66	125.04
5	A	1001	HEA	CAD-C3D-C4D	2.35	128.76	124.66
5	E	1002	HEA	C4C-NC-C1C	-2.34	103.05	105.35
5	A	1002	HEA	C4C-NC-C1C	-2.34	103.06	105.35
5	E	1001	HEA	CMD-C2D-C1D	2.34	128.60	125.04
5	E	1002	HEA	CMD-C2D-C1D	2.33	128.59	125.04
7	A	1004	MQ7	C2M-C2-C3	-2.30	120.64	124.40
7	E	1004	MQ7	C2M-C2-C3	-2.30	120.65	124.40
5	A	1001	HEA	CHB-C4A-NA	-2.29	121.96	124.44
5	E	1001	HEA	CHB-C4A-NA	-2.29	121.96	124.44
5	A	1002	HEA	CHB-C4A-NA	-2.27	121.99	124.44
5	A	1002	HEA	CAD-C3D-C4D	2.23	128.56	124.66
5	E	1002	HEA	CHB-C4A-NA	-2.19	122.07	124.44
5	E	1002	HEA	CHD-C1D-C2D	-2.13	120.82	126.73
5	A	1002	HEA	CHD-C1D-C2D	-2.08	120.96	126.73
5	A	1001	HEA	OMA-CMA-C3A	-2.06	121.02	125.69
5	E	1001	HEA	C13-C12-C11	-2.05	111.26	114.35
5	E	1002	HEA	OMA-CMA-C3A	-2.05	121.05	125.69
5	A	1002	HEA	OMA-CMA-C3A	-2.04	121.07	125.69
5	A	1001	HEA	CAD-CBD-CGD	-2.03	109.25	113.60
5	E	1001	HEA	OMA-CMA-C3A	-2.01	121.15	125.69

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	HEA	C2A-C3A-CMA-OMA
5	A	1001	HEA	C4A-C3A-CMA-OMA
5	A	1001	HEA	C3B-C11-C12-C13
5	A	1001	HEA	O11-C11-C12-C13
5	E	1001	HEA	C2A-C3A-CMA-OMA
5	E	1001	HEA	C4A-C3A-CMA-OMA
5	E	1001	HEA	C3B-C11-C12-C13
5	E	1001	HEA	O11-C11-C12-C13
5	A	1001	HEA	C15-C16-C17-C18
5	E	1001	HEA	C15-C16-C17-C18
7	A	1004	MQ7	C17-C18-C20-C21
7	A	1004	MQ7	C19-C18-C20-C21
7	E	1004	MQ7	C19-C18-C20-C21
7	E	1004	MQ7	C17-C18-C20-C21
7	A	1004	MQ7	C24-C23-C25-C26
7	E	1004	MQ7	C24-C23-C25-C26
7	A	1004	MQ7	C22-C23-C25-C26
7	E	1004	MQ7	C22-C23-C25-C26
5	A	1001	HEA	C26-C15-C16-C17
5	E	1001	HEA	C26-C15-C16-C17
5	A	1001	HEA	C14-C15-C16-C17
5	E	1001	HEA	C14-C15-C16-C17
5	A	1002	HEA	C2A-C3A-CMA-OMA
5	E	1002	HEA	C2A-C3A-CMA-OMA
5	A	1002	HEA	C4A-C3A-CMA-OMA
5	E	1002	HEA	C4A-C3A-CMA-OMA
7	E	1004	MQ7	C14-C13-C15-C16
7	A	1004	MQ7	C14-C13-C15-C16
5	A	1001	HEA	C19-C20-C21-C22
5	E	1001	HEA	C19-C20-C21-C22
5	A	1001	HEA	C2A-CAA-CBA-CGA
5	E	1001	HEA	C2A-CAA-CBA-CGA
5	E	1002	HEA	CAD-CBD-CGD-O1D
5	A	1002	HEA	CAD-CBD-CGD-O1D
5	E	1002	HEA	CAD-CBD-CGD-O2D
5	A	1002	HEA	CAD-CBD-CGD-O2D
7	E	1004	MQ7	C12-C13-C15-C16
5	E	1002	HEA	CAA-CBA-CGA-O2A
5	A	1002	HEA	CAA-CBA-CGA-O2A
7	A	1004	MQ7	C12-C13-C15-C16
5	A	1002	HEA	C2D-C3D-CAD-CBD
5	E	1002	HEA	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
5	A	1002	HEA	CAA-CBA-CGA-O1A
5	E	1002	HEA	CAA-CBA-CGA-O1A
5	A	1002	HEA	C26-C15-C16-C17
5	E	1002	HEA	C26-C15-C16-C17
5	A	1001	HEA	CAD-CBD-CGD-O2D
5	E	1001	HEA	CAD-CBD-CGD-O2D
5	A	1001	HEA	CAA-CBA-CGA-O1A
5	E	1001	HEA	CAA-CBA-CGA-O1A
5	E	1001	HEA	CAD-CBD-CGD-O1D
5	A	1002	HEA	C4D-C3D-CAD-CBD
5	E	1002	HEA	C4D-C3D-CAD-CBD
5	A	1001	HEA	CAD-CBD-CGD-O1D
5	E	1001	HEA	CAA-CBA-CGA-O2A
5	A	1001	HEA	CAA-CBA-CGA-O2A

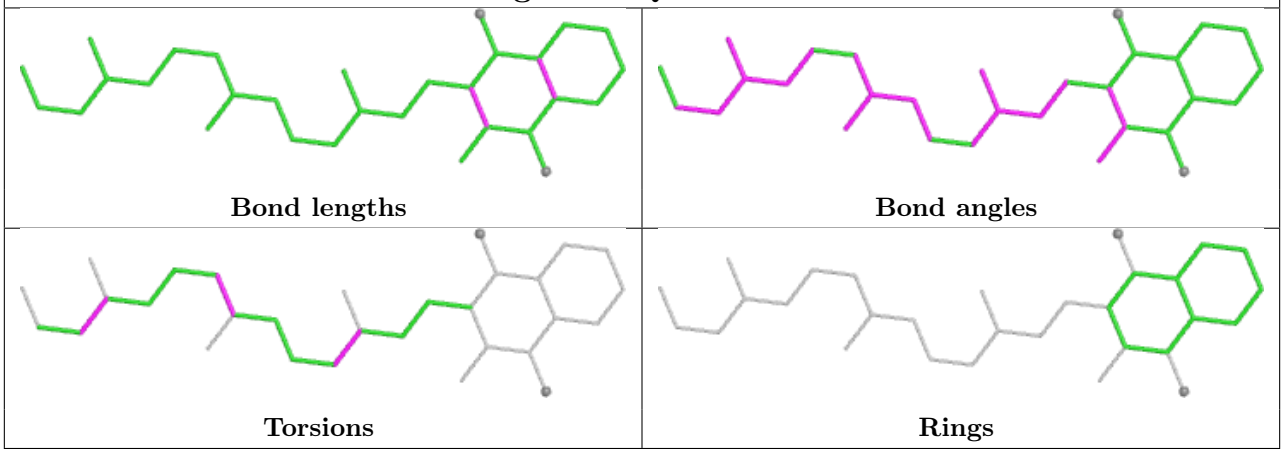
There are no ring outliers.

6 monomers are involved in 27 short contacts:

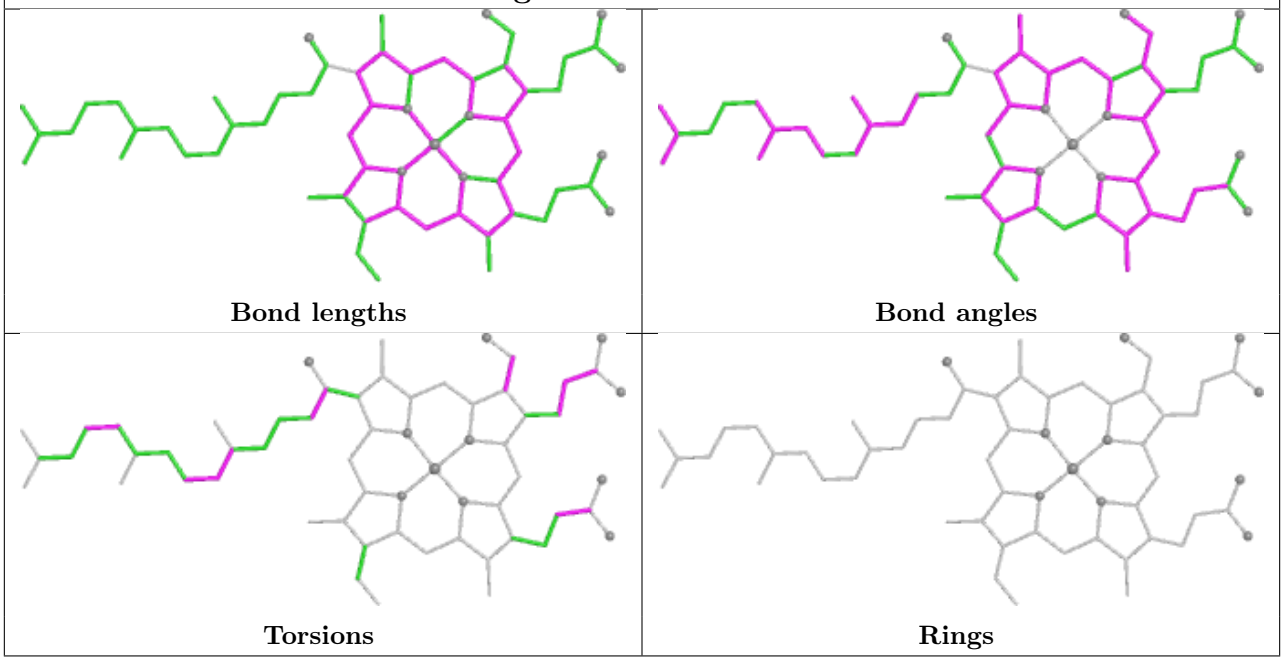
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1004	MQ7	1	0
5	A	1001	HEA	6	0
5	A	1002	HEA	7	0
7	E	1004	MQ7	1	0
5	E	1001	HEA	5	0
5	E	1002	HEA	7	0

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 then 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.

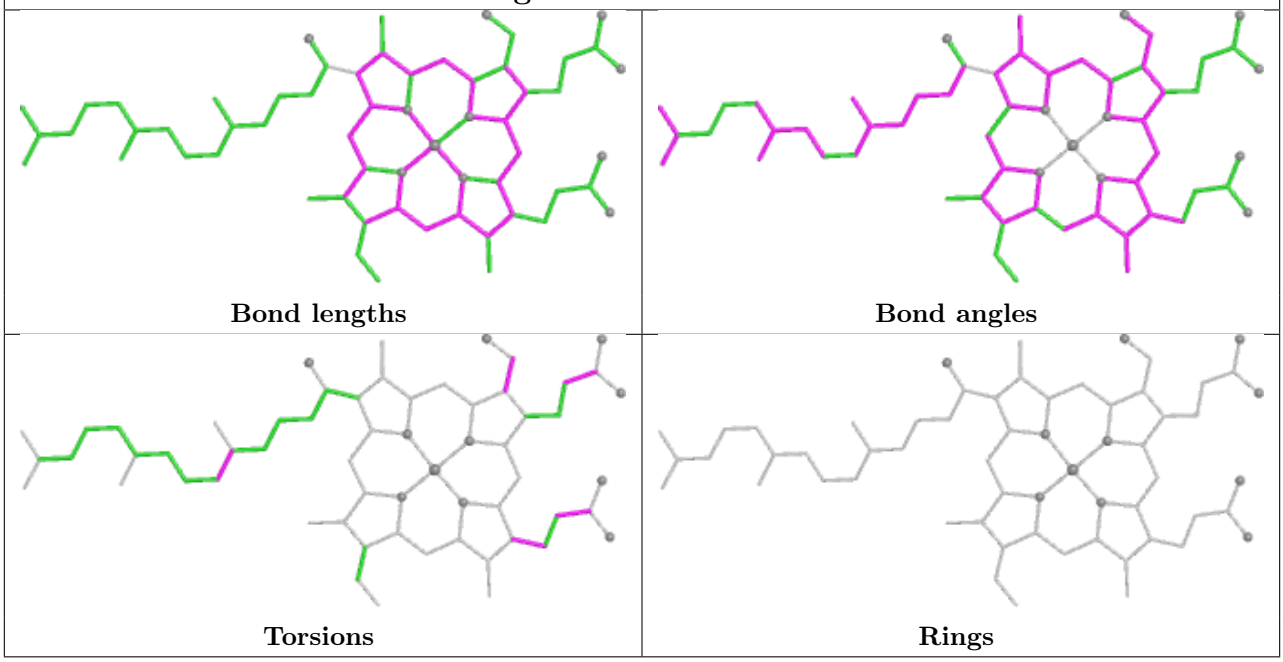
Ligand MQ7 A 1004



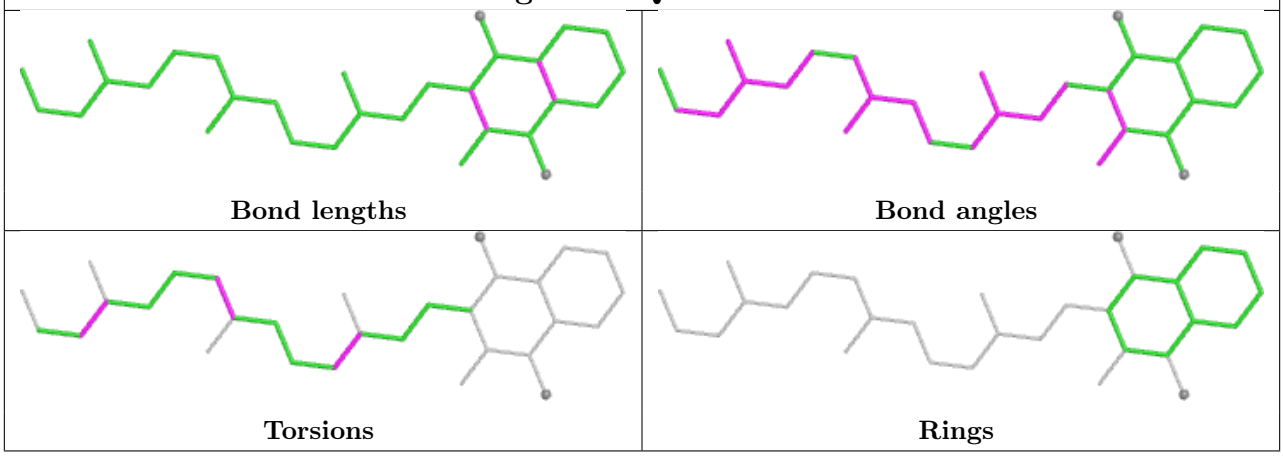
Ligand HEA A 1001



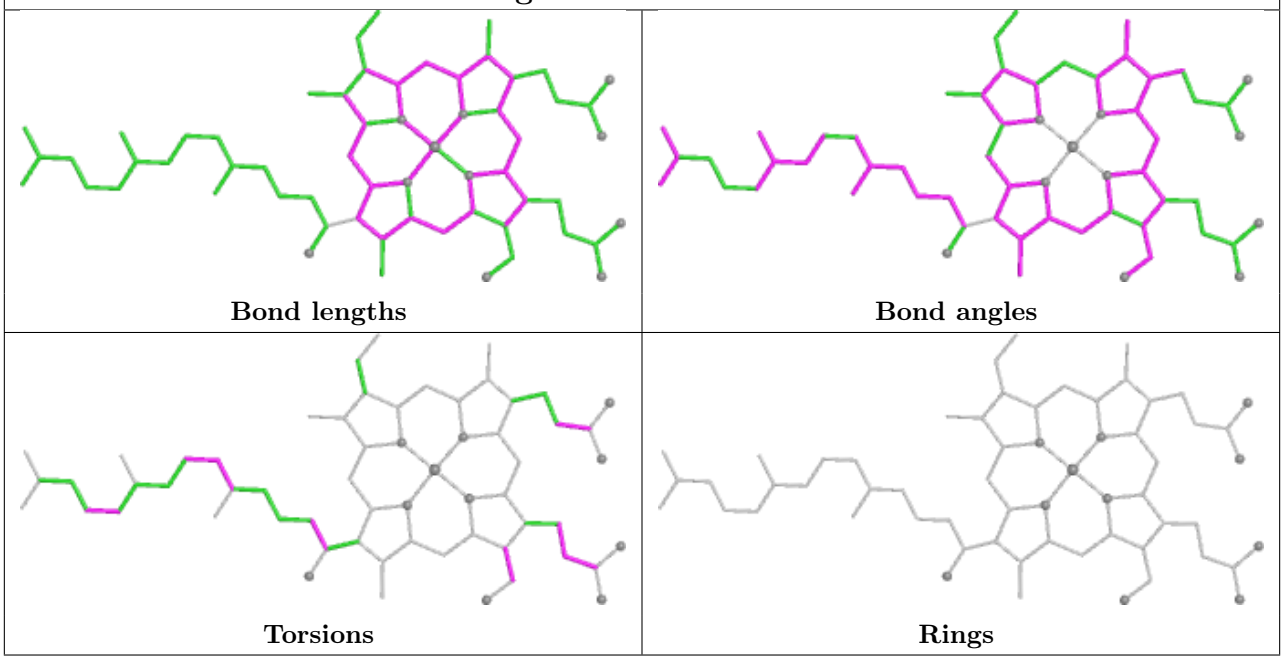
Ligand HEA A 1002



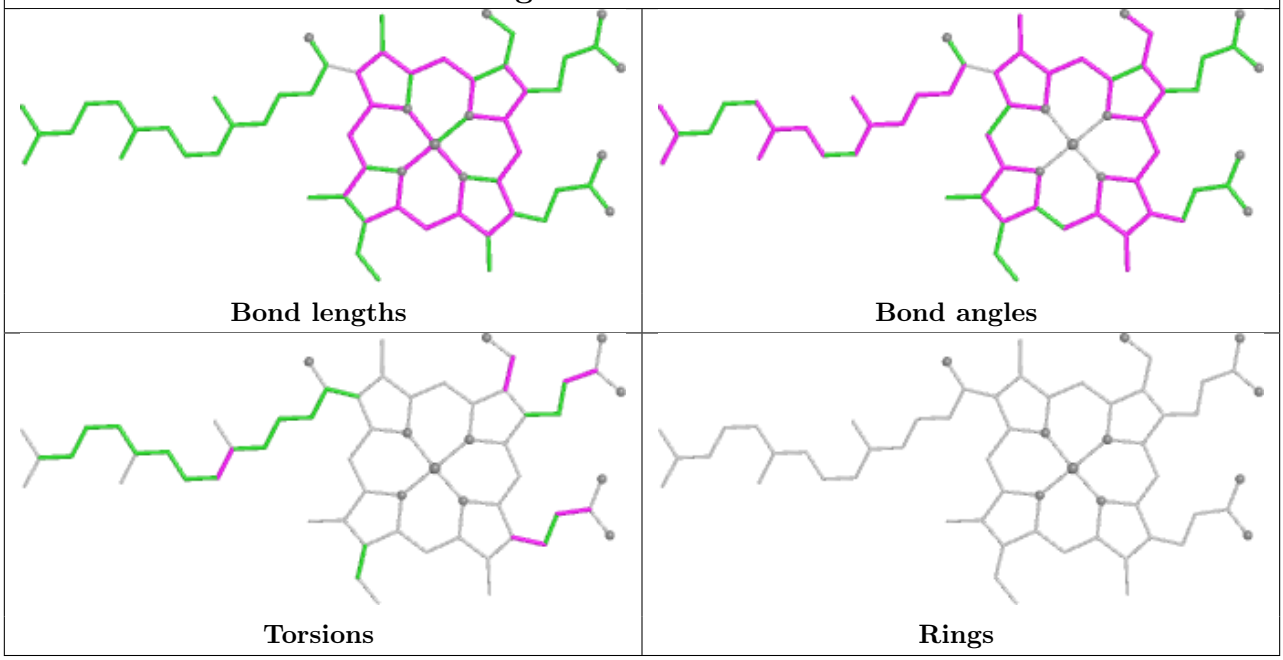
Ligand MQ7 E 1004



Ligand HEA E 1001



Ligand HEA E 1002



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.99	85 (14%)	6	6	56, 118, 176, 223	0
1	E	607/655 (92%)	1.20	125 (20%)	2	3	68, 127, 201, 269	0
2	B	256/296 (86%)	1.07	45 (17%)	4	4	72, 151, 205, 238	0
2	F	256/296 (86%)	1.08	48 (18%)	3	3	70, 147, 210, 258	0
3	C	178/204 (87%)	1.06	22 (12%)	8	7	72, 125, 188, 237	0
3	G	178/204 (87%)	1.15	28 (15%)	5	5	75, 134, 203, 230	0
4	D	48/124 (38%)	0.91	8 (16%)	4	5	84, 126, 172, 190	0
4	H	48/124 (38%)	1.12	11 (22%)	2	2	73, 122, 174, 191	0
All	All	2178/2558 (85%)	1.09	372 (17%)	4	4	56, 130, 199, 269	0

All (372) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	486	ASP	7.4
3	G	53	ALA	7.3
1	E	333	THR	6.9
2	F	253	GLY	6.6
3	G	181	TYR	6.5
2	B	274	HIS	6.4
2	B	73	VAL	5.8
1	A	93	ASN	5.7
3	G	34	GLU	5.6
3	G	124	GLU	5.5
1	E	128	GLY	5.4
1	E	240	PRO	5.3
1	A	86	ASN	5.2
1	A	58	ILE	5.2
2	F	169	LEU	5.2
2	F	156	PRO	4.9

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Mol	Chain	Res	Type	RSRZ
1	E	174	SER	4.9
3	G	37	LEU	4.9
1	A	163	ASN	4.8
3	G	54	GLY	4.7
1	A	432	PHE	4.7
1	A	437	PRO	4.7
3	G	50	ASN	4.6
4	D	69	GLU	4.6
1	E	357	VAL	4.6
3	C	119	VAL	4.6
4	H	70	ASN	4.6
2	F	19	ASP	4.6
1	E	199	MET	4.5
2	B	188	ASN	4.5
1	E	405	GLN	4.4
3	G	144	HIS	4.4
1	E	440	PHE	4.4
1	E	614	GLY	4.3
2	B	190	THR	4.3
2	F	159	GLY	4.3
3	G	52	THR	4.2
1	E	164	ALA	4.2
1	A	438	LYS	4.2
1	E	473	GLN	4.1
1	E	480	TYR	4.1
2	F	23	LEU	4.1
2	B	283	VAL	4.1
1	A	52	ASP	4.1
3	C	74	LEU	4.1
3	C	53	ALA	4.1
3	G	90	ARG	4.0
1	E	441	GLY	4.0
2	B	235	GLU	4.0
3	C	80	THR	4.0
1	E	105	ILE	4.0
1	E	305	GLN	4.0
2	B	70	VAL	3.9
2	B	160	GLY	3.9
1	E	158	ILE	3.9
2	F	115	TRP	3.9
3	C	116	ASN	3.8
1	E	504	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	282	ASN	3.8
1	E	34	LEU	3.8
1	E	408	ASN	3.8
3	C	120	HIS	3.7
2	F	30	PHE	3.7
1	E	296	GLU	3.7
1	E	406	TYR	3.7
1	A	54	LYS	3.7
1	E	95	TYR	3.7
1	A	167	THR	3.6
1	E	136	TYR	3.6
1	A	317	ILE	3.6
1	A	178	SER	3.6
1	A	327	TRP	3.6
2	B	97	PRO	3.6
1	A	240	PRO	3.5
1	E	412	LEU	3.5
1	E	609	TRP	3.5
1	A	313	VAL	3.5
1	E	32	PHE	3.5
1	A	61	ILE	3.4
1	A	578	LYS	3.4
1	E	515	TYR	3.4
2	F	168	MET	3.4
1	E	516	SER	3.4
1	A	541	SER	3.4
3	C	126	ALA	3.4
2	B	258	TYR	3.4
1	E	332	PHE	3.4
1	E	587	GLY	3.4
1	A	386	ASN	3.4
1	A	55	LYS	3.3
1	E	263	GLU	3.3
1	A	350	ALA	3.3
1	E	224	PHE	3.3
1	E	445	ASN	3.3
4	D	70	ASN	3.3
1	A	128	GLY	3.3
1	E	487	GLY	3.3
1	E	311	ALA	3.3
1	E	613	VAL	3.2
1	A	430	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	243	THR	3.2
1	E	584	SER	3.2
2	B	236	ASN	3.2
4	D	60	LEU	3.2
2	F	189	PHE	3.2
1	E	79	ARG	3.2
1	E	303	ARG	3.2
4	H	63	MET	3.2
3	C	81	CYS	3.2
2	B	234	PRO	3.2
1	A	579	LYS	3.2
3	C	97	VAL	3.2
1	A	164	ALA	3.1
2	B	92	SER	3.1
2	B	259	ALA	3.1
1	A	491	LEU	3.1
1	A	314	GLY	3.1
1	E	269	MET	3.1
1	A	165	GLY	3.1
2	F	236	ASN	3.1
1	E	321	VAL	3.1
1	E	127	ILE	3.1
1	E	596	PHE	3.1
2	F	264	LYS	3.1
2	B	191	GLY	3.1
1	A	238	ALA	3.1
1	A	48	ILE	3.0
1	A	121	VAL	3.0
2	F	191	GLY	3.0
1	E	537	TRP	3.0
3	C	124	GLU	3.0
1	A	540	SER	3.0
1	E	585	ASN	3.0
1	E	314	GLY	3.0
3	C	136	GLY	3.0
1	E	580	ILE	3.0
2	B	277	THR	3.0
1	E	211	MET	2.9
1	E	461	ASN	2.9
1	E	162	PRO	2.9
2	F	226	GLU	2.9
4	H	69	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	165	GLY	2.9
2	F	160	GLY	2.9
3	G	172	SER	2.9
2	B	252	HIS	2.9
1	E	51	VAL	2.9
1	E	558	GLN	2.9
1	A	305	GLN	2.9
2	B	16	GLN	2.9
3	G	82	GLY	2.9
1	A	298	ILE	2.9
1	E	421	ILE	2.9
1	A	321	VAL	2.8
1	A	15	LEU	2.8
1	A	487	GLY	2.8
1	A	543	ILE	2.8
1	E	196	GLY	2.8
2	F	254	GLN	2.8
4	D	95	ILE	2.8
2	B	154	TRP	2.8
1	E	418	TYR	2.8
1	A	416	PHE	2.8
1	E	175	ASN	2.8
1	E	295	SER	2.8
2	F	109	TYR	2.8
1	A	492	ASN	2.8
2	F	16	GLN	2.8
3	G	30	PHE	2.8
1	A	361	ASN	2.8
2	F	224	THR	2.8
3	G	33	ALA	2.8
4	H	72	THR	2.8
2	F	251	ASP	2.7
1	A	428	CYS	2.7
3	G	91	GLY	2.7
1	E	35	THR	2.7
1	A	488	TRP	2.7
1	A	179	PRO	2.7
2	F	249	TYR	2.7
3	G	126	ALA	2.7
1	E	178	SER	2.7
1	A	62	ILE	2.7
1	E	404	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	482	TYR	2.7
3	G	127	ALA	2.7
1	E	222	PRO	2.7
1	E	468	TYR	2.7
1	E	568	LYS	2.7
1	A	495	SER	2.7
3	C	171	THR	2.6
1	A	281	PRO	2.6
1	A	439	MET	2.6
1	E	536	ASP	2.6
1	E	331	PHE	2.6
1	E	15	LEU	2.6
2	B	279	PRO	2.6
1	E	530	GLY	2.6
2	B	120	SER	2.6
2	B	50	LYS	2.6
1	E	488	TRP	2.5
2	F	276	LYS	2.5
1	A	469	PHE	2.5
2	F	187	ALA	2.5
4	D	58	GLN	2.5
1	E	308	GLY	2.5
3	G	142	GLY	2.5
4	H	71	GLY	2.5
1	A	296	GLU	2.5
1	E	33	VAL	2.5
1	A	47	TRP	2.5
1	E	192	ILE	2.5
1	E	304	LYS	2.5
2	F	167	GLY	2.5
1	E	557	SER	2.5
2	F	22	LEU	2.5
2	F	149	SER	2.5
3	G	143	THR	2.5
1	E	244	VAL	2.5
2	F	94	GLU	2.5
2	F	171	ASP	2.5
3	C	127	ALA	2.4
1	A	408	ASN	2.4
1	E	264	ALA	2.4
1	A	117	GLY	2.4
1	E	439	MET	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	250	VAL	2.4
2	B	163	TYR	2.4
1	E	485	ASN	2.4
2	F	18	SER	2.4
1	E	460	PHE	2.4
4	H	95	ILE	2.4
1	A	280	HIS	2.4
1	A	466	PRO	2.4
3	G	74	LEU	2.4
2	B	17	GLN	2.4
1	E	194	GLY	2.4
2	F	282	ASN	2.4
3	G	154	TRP	2.4
1	E	161	SER	2.4
3	C	78	SER	2.4
1	A	355	THR	2.4
1	E	535	LEU	2.4
2	F	106	LEU	2.4
1	E	279	GLY	2.3
4	H	83	PHE	2.3
1	E	306	LEU	2.3
1	E	238	ALA	2.3
1	E	92	SER	2.3
3	C	20	GLY	2.3
3	G	92	SER	2.3
1	E	139	ASN	2.3
2	B	187	ALA	2.3
1	E	606	GLU	2.3
2	F	114	ASP	2.3
1	E	416	PHE	2.3
1	E	598	LEU	2.3
3	C	77	SER	2.3
2	F	154	TRP	2.3
2	B	150	MET	2.3
2	B	276	LYS	2.3
1	E	168	SER	2.3
1	A	431	GLY	2.3
2	B	181	THR	2.3
2	B	115	TRP	2.3
2	B	162	LYS	2.3
1	A	405	GLN	2.3
1	E	446	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	474	GLY	2.3
1	A	205	MET	2.3
2	F	188	ASN	2.3
1	A	449	GLY	2.3
3	C	55	GLY	2.3
3	G	26	GLY	2.3
1	E	478	ARG	2.3
3	G	51	ARG	2.3
1	E	415	HIS	2.2
1	A	287	ILE	2.2
2	B	76	ILE	2.2
2	F	259	ALA	2.2
2	F	150	MET	2.2
3	G	89	ARG	2.2
1	E	397	LEU	2.2
1	E	96	ASN	2.2
2	B	186	ASN	2.2
1	A	434	PHE	2.2
1	A	169	TYR	2.2
1	A	14	PRO	2.2
4	H	82	PHE	2.2
2	F	268	TYR	2.2
4	H	92	SER	2.2
2	B	69	VAL	2.2
3	C	54	GLY	2.2
1	E	101	THR	2.2
2	B	224	THR	2.2
3	C	133	PHE	2.2
1	E	203	ASN	2.2
1	A	166	TRP	2.2
1	E	267	MET	2.2
1	A	118	LEU	2.2
1	A	608	TYR	2.2
1	E	477	ARG	2.2
2	B	249	TYR	2.2
2	B	108	VAL	2.2
1	A	606	GLU	2.2
1	E	476	PRO	2.2
1	E	566	GLU	2.2
2	B	94	GLU	2.2
3	C	130	THR	2.2
4	D	63	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	451	TRP	2.2
3	G	99	TRP	2.2
3	G	189	TRP	2.2
1	E	368	LYS	2.2
2	B	153	LEU	2.2
2	F	260	MET	2.2
4	H	79	LEU	2.2
2	B	159	GLY	2.1
4	H	49	GLY	2.1
2	B	192	GLU	2.1
2	F	190	THR	2.1
1	A	412	LEU	2.1
1	E	223	MET	2.1
1	E	372	SER	2.1
2	F	272	SER	2.1
1	E	559	ASP	2.1
1	E	392	VAL	2.1
2	F	237	VAL	2.1
1	A	136	TYR	2.1
2	B	241	THR	2.1
3	C	52	THR	2.1
1	E	552	LEU	2.1
1	A	542	ALA	2.1
1	A	168	SER	2.1
2	B	18	SER	2.1
1	A	482	TYR	2.1
1	E	322	LEU	2.1
3	G	170	GLN	2.1
1	A	276	TRP	2.1
2	F	163	TYR	2.1
1	E	589	PRO	2.1
1	E	144	THR	2.1
2	F	83	SER	2.1
2	F	222	LYS	2.1
2	B	157	GLN	2.1
1	A	435	TRP	2.1
1	E	327	TRP	2.1
1	A	225	THR	2.1
1	A	318	ALA	2.1
1	E	146	PHE	2.1
4	D	80	PHE	2.1
1	A	79	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	478	ARG	2.0
1	A	277	ILE	2.0
3	C	24	ILE	2.0
1	E	307	PHE	2.0
1	A	21	VAL	2.0
2	F	215	LYS	2.0
4	D	78	THR	2.0
1	E	567	GLU	2.0
1	A	605	PHE	2.0
1	E	290	ALA	2.0
2	B	161	GLN	2.0
1	A	203	ASN	2.0
1	A	476	PRO	2.0
2	F	274	HIS	2.0
1	E	401	ALA	2.0
1	E	586	SER	2.0
1	A	392	VAL	2.0
1	E	157	VAL	2.0
1	E	395	VAL	2.0
2	F	44	VAL	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(Å^2)	Q<0.9
7	MQ7	E	1004	30/48	0.73	0.30	176,203,224,225	0
6	CU	A	1003	1/1	0.79	0.14	169,169,169,169	0
7	MQ7	A	1004	30/48	0.82	0.20	121,147,178,189	0

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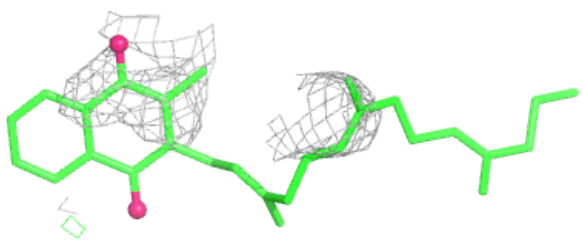
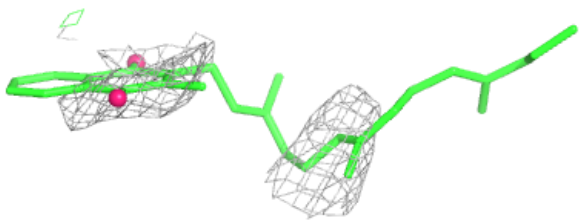
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CU	E	1003	1/1	0.91	0.08	122,122,122,122	0
5	HEA	A	1002	60/60	0.92	0.23	68,147,209,219	0
5	HEA	E	1002	60/60	0.92	0.23	97,140,157,163	0
5	HEA	A	1001	60/60	0.92	0.22	74,125,158,169	0
5	HEA	E	1001	60/60	0.93	0.21	66,114,186,214	0

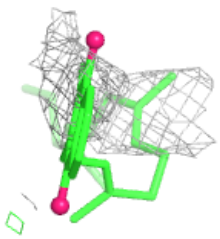
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MQ7 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)

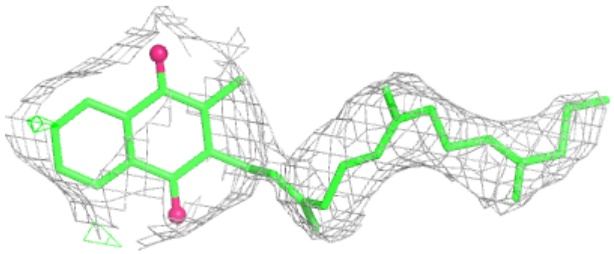


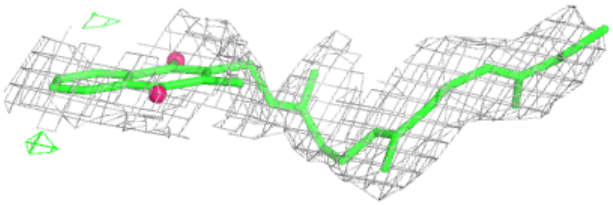


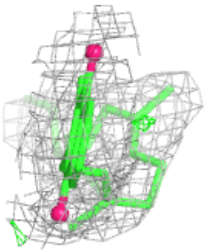


Electron density around MQ7 A 1004:

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

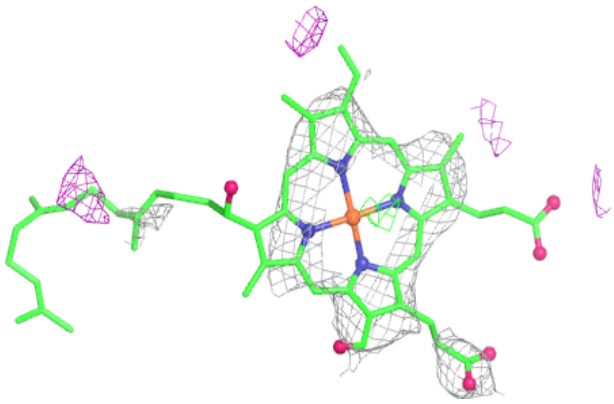


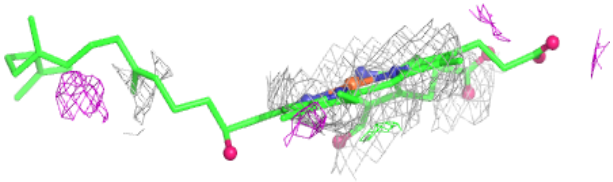


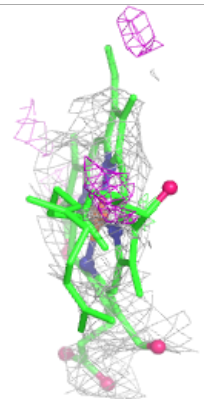


Electron density around HEA A 1002:

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

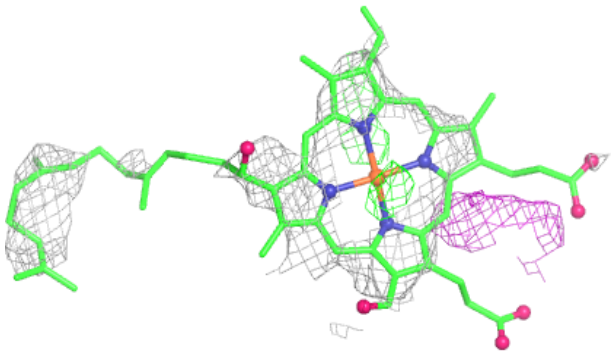


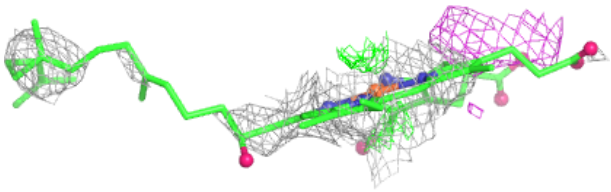


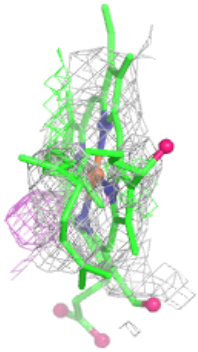


Electron density around HEA E 1002:

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

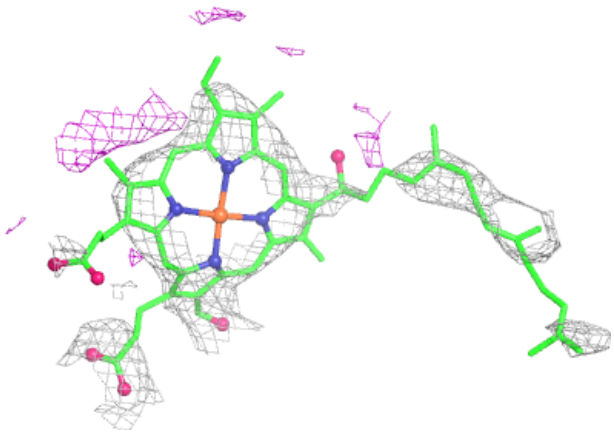


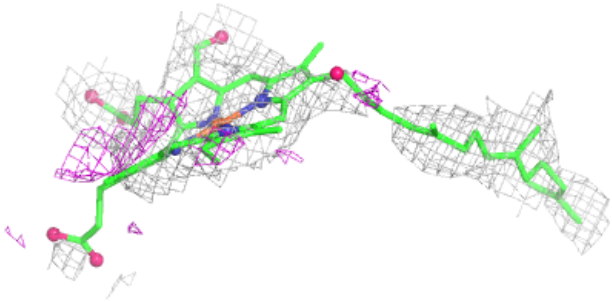


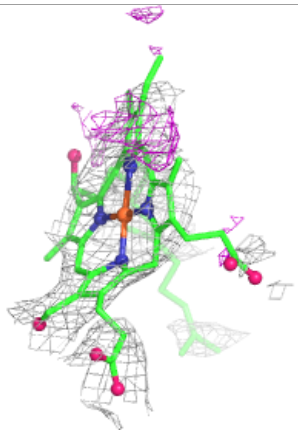


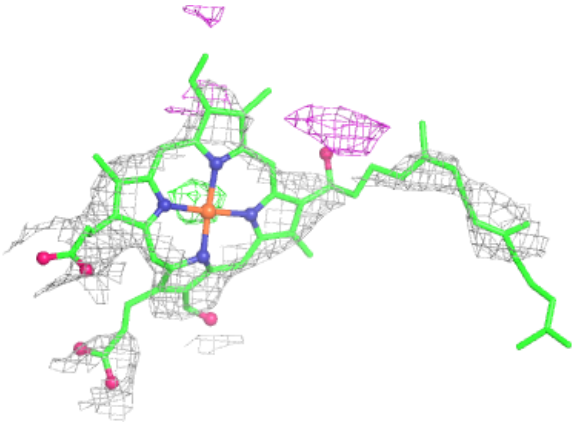
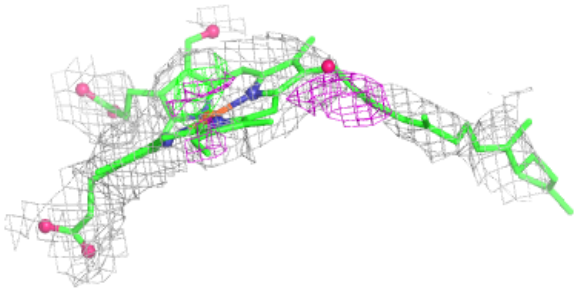
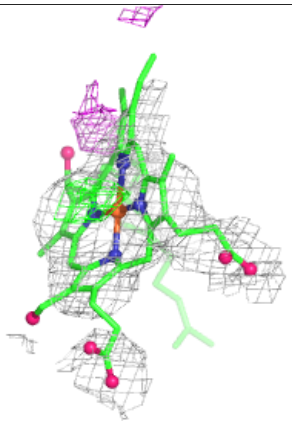
Electron density around HEA A 1001:

$2mF_o$-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.