



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2026 – 05:08 am BST

PDB ID : 2YEV / pdb_00002yev
Title : Structure of caa3-type cytochrome oxidase
Authors : Lyons, J.A.; Aragao, D.; Soulimane, T.; Caffrey, M.
Deposited on : 2011-03-31
Resolution : 2.36 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	:	1.8.4, 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

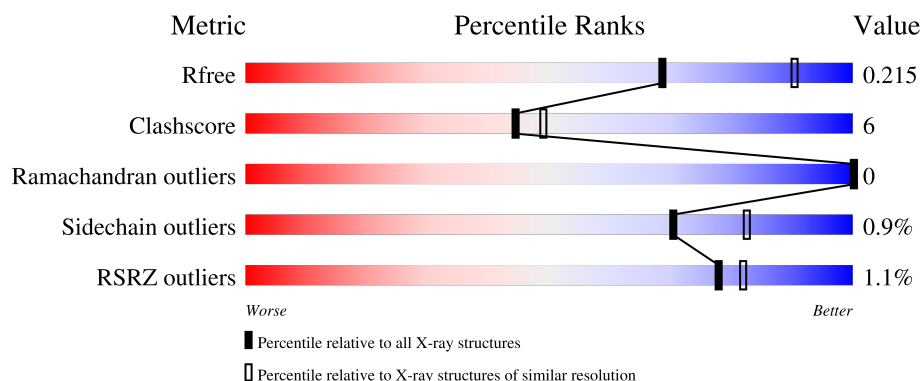
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	791	6% 85% 14% .
1	D	791	6% 84% 14% .
2	B	337	83% 11% 5%
2	E	337	6% 82% 12% . 5%
3	C	66	6% 85% 12% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	66	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	HEC	B	587	X	-	-	-
11	HEC	E	587	X	-	-	-
5	HAS	A	1015	X	-	-	-
5	HAS	A	1016	X	-	-	-
5	HAS	D	1015	X	-	-	-
5	HAS	D	1016	X	-	-	-
8	7E8	A	1300	X	-	-	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 19587 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 CYTOCHROME C OXIDASE POLYPEPTIDE I+III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	780	Total	C	N	O	S	0	1	0
			6281	4244	992	1022	23			
1	D	780	Total	C	N	O	S	0	0	0
			6276	4241	992	1020	23			

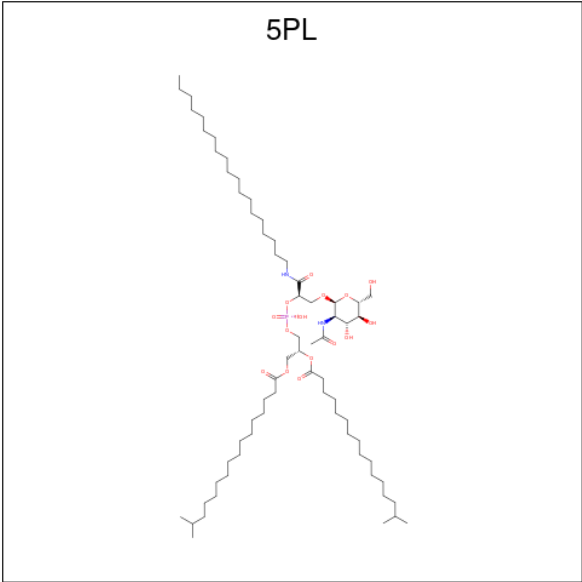
- Molecule 2 is a protein called CYTOCHROME C OXIDASE SUBUNIT 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	319	Total	C	N	O	S	0	0	0
			2507	1637	422	439	9			
2	E	319	Total	C	N	O	S	0	0	0
			2507	1637	422	439	9			

- Molecule 3 is a protein called CAA3-TYPE CYTOCHROME OXIDASE SUBUNIT IV.

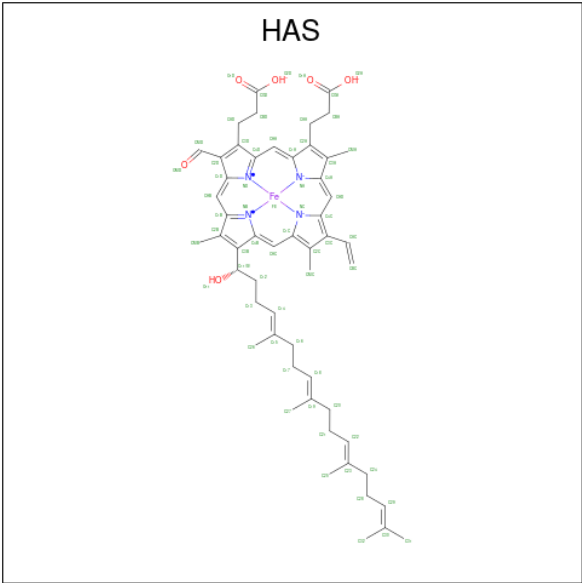
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	64	Total	C	N	O	S	0	0	0
			502	344	76	79	3			
3	F	63	Total	C	N	O	S	0	0	0
			492	338	73	78	3			

- Molecule 4 is (1R,4S,6R)-6-({[2-(ACETYLAMINO)-2-DEOXY-ALPHA-D-GLUCOPYRANOSYL]OXY}METHYL)-4-HYDROXY-1-[[[(15-METHYLHEXADECANOYL)OXY]METHYL]-4-OXIDO-7-OXO-3,5-DIOXA-8-AZA-4-PHOSPHAHEPTACOS-1-YL 15-METHYLHEXADECANOATE (CCD ID: 5PL) (formula: C₆₇H₁₂₉N₂O₁₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			85	67	2	15	1		
4	D	1	Total	C	N	O	P	0	0
			85	67	2	15	1		

- Molecule 5 is HEME-AS (CCD ID: HAS) (formula: C₅₄H₆₄FeN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			65	54	1	4	6		
5	A	1	Total	C	Fe	N	O	0	0
			65	54	1	4	6		

Continued on next page...

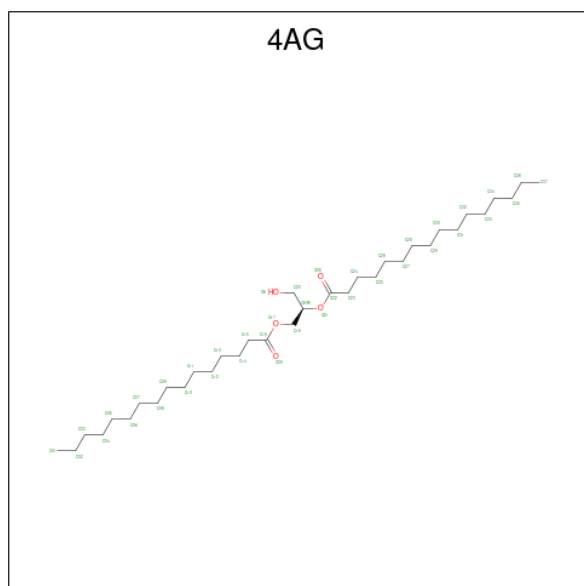
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	Fe	N	O	
			65	54	1	4	6	
5	D	1	Total	C	Fe	N	O	
			65	54	1	4	6	

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

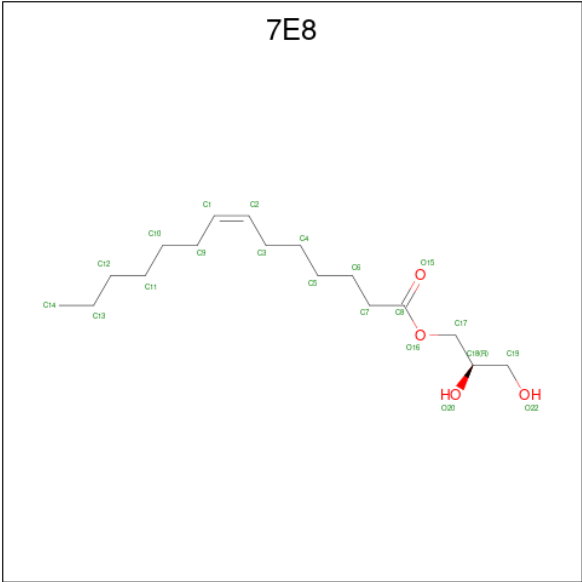
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cu		
			1	1	0	0
6	D	1	Total	Cu		
			1	1	0	0

- Molecule 7 is (2R)-3-HYDROXYPROPANE-1,2-DIYL DIHEXADECANOATE (CCD ID: 4AG) (formula: C₃₅H₆₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O		
			40	35	5	0	0

- Molecule 8 is (2R)-2,3-DIHYDROXYPROPYL (7Z)-TETRADEC-7-ENOATE (CCD ID: 7E8) (formula: C₁₇H₃₂O₄).

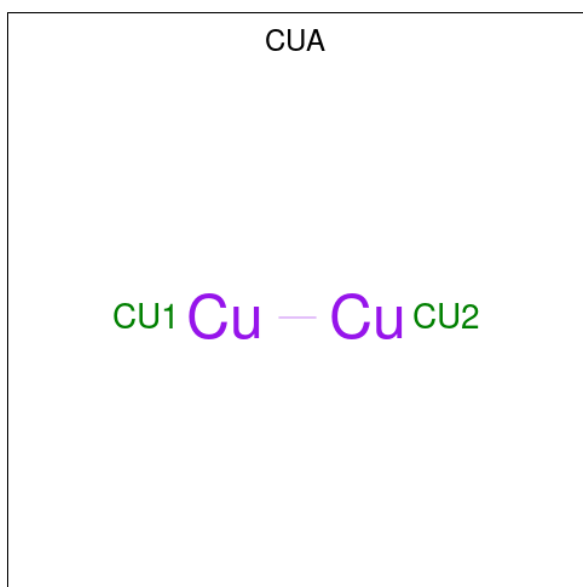


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			21	17	4		
8	A	1	Total	C	O	0	0
			21	17	4		

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

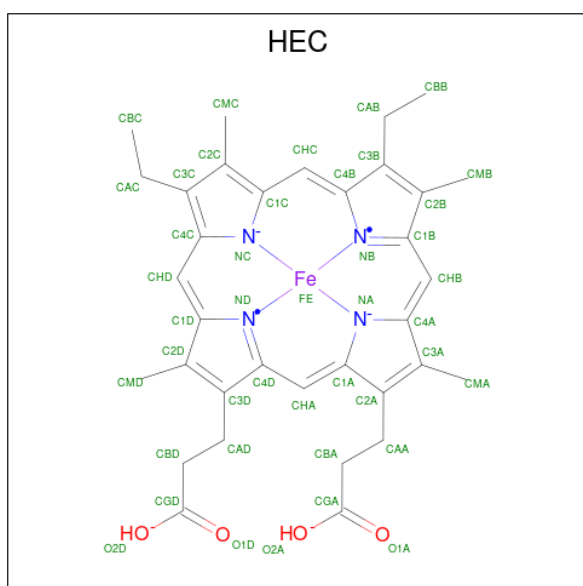
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Mg	0	0
			1	1		
9	D	1	Total	Mg	0	0
			1	1		

- Molecule 10 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



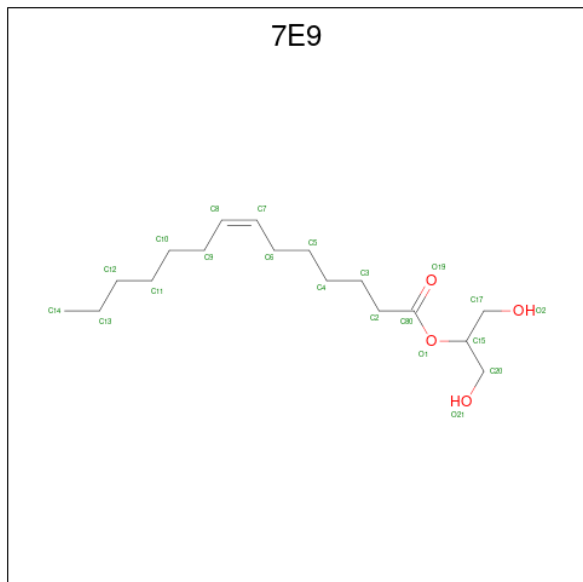
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Cu 2 2	0	0
10	E	1	Total Cu 2 2	0	0

- Molecule 11 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
11	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 12 is 1,3-DIHYDROXYPROPAN-2-YL (Z)-TETRADEC-7-ENOATE (CCD ID: 7E9) (formula: C₁₇H₃₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	0
			21	17	4		

- Molecule 13 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	1	Total	Cl	0	0
			1	1		
13	D	1	Total	Cl	0	0
			1	1		
13	F	1	Total	Cl	0	0
			1	1		

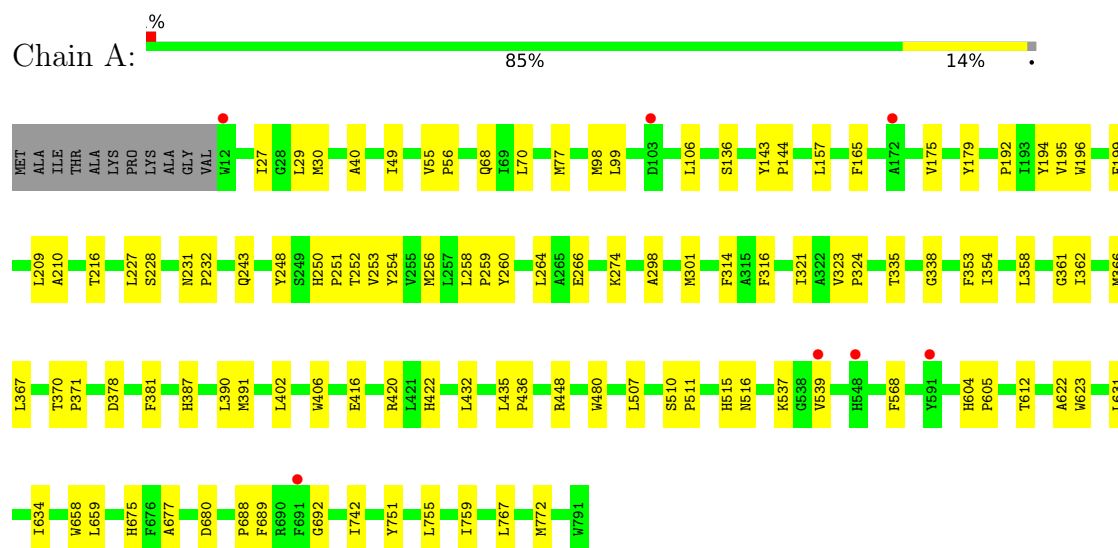
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	157	Total	O	0	0
			157	157		
14	B	90	Total	O	0	0
			90	90		
14	D	111	Total	O	0	0
			111	111		
14	E	34	Total	O	0	0
			34	34		

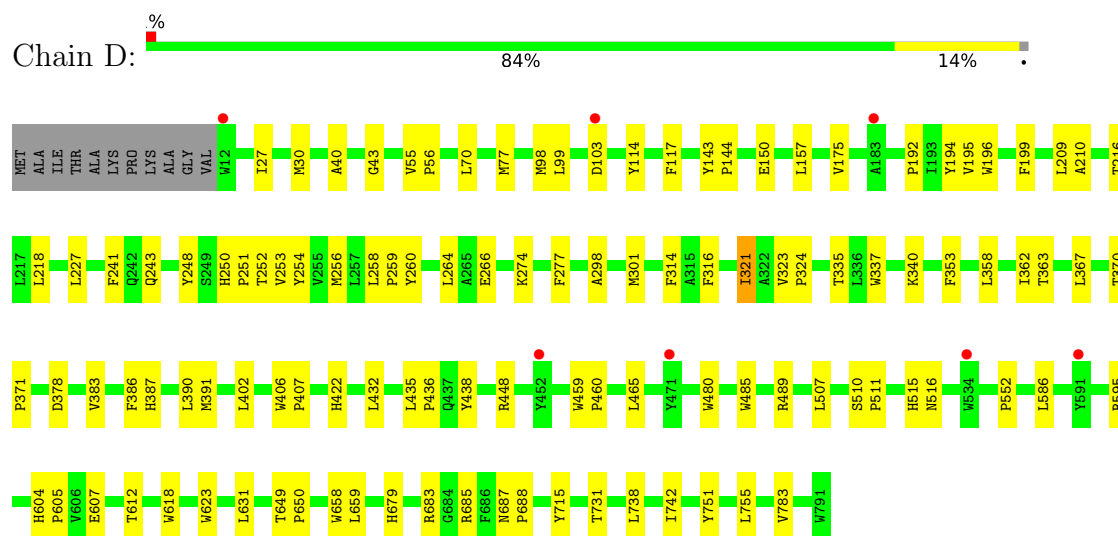
3 Residue-property plots [i](#)

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.

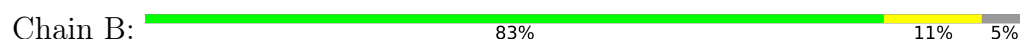
• Molecule 1: CYTOCHROME C OXIDASE POLYPEPTIDE I+III

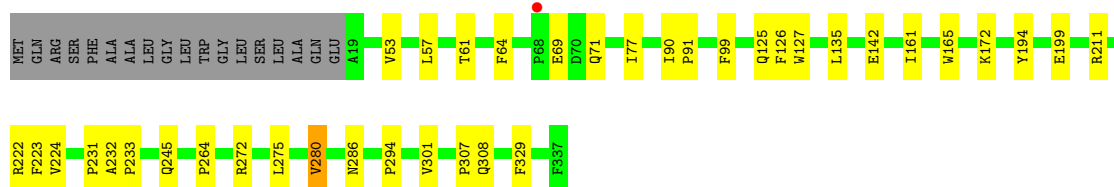


• Molecule 1: CYTOCHROME C OXIDASE POLYPEPTIDE I+III

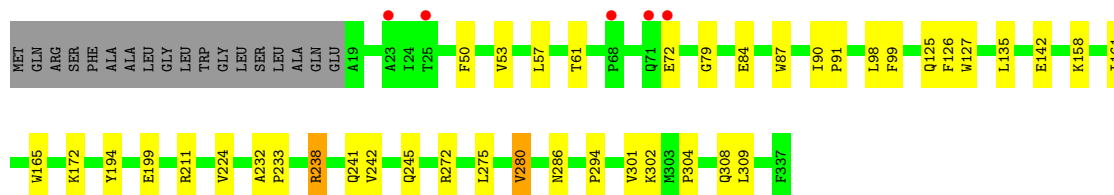
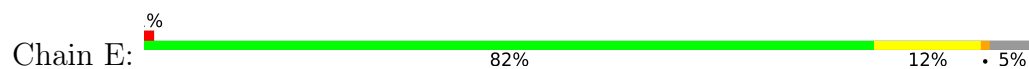


• Molecule 2: CYTOCHROME C OXIDASE SUBUNIT 2

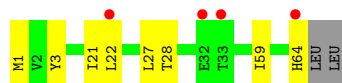
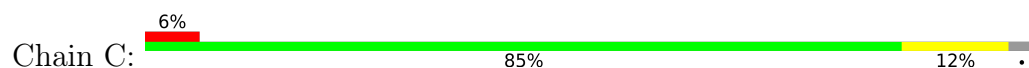




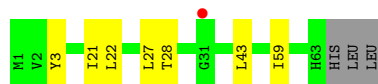
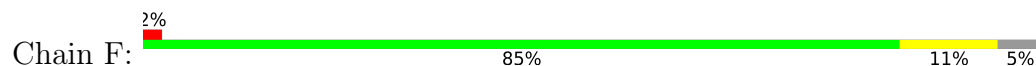
• Molecule 2: CYTOCHROME C OXIDASE SUBUNIT 2



• Molecule 3: CAA3-TYPE CYTOCHROME OXIDASE SUBUNIT IV



• Molecule 3: CAA3-TYPE CYTOCHROME OXIDASE SUBUNIT IV



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	127.25Å 76.03Å 300.27Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	77.18 – 2.36 77.18 – 2.36	Depositor EDS
% Data completeness (in resolution range)	100.0 (77.18-2.36) 100.0 (77.18-2.36)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.37Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.4_486)	Depositor
R, R_{free}	0.171 , 0.218 0.168 , 0.215	Depositor DCC
R_{free} test set	5970 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19587	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: CL, CU, 5PL, HAS, CUA, MG, FME, 7E9, 4AG, 7E8, HEC

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	0.39	0/6523	0.70	0/8921
1	D	0.39	0/6515	0.70	0/8910
2	B	0.41	0/2586	0.74	0/3523
2	E	0.38	0/2586	0.75	0/3523
3	C	0.34	0/502	0.65	0/683
3	F	0.35	0/491	0.67	0/668
All	All	0.39	0/19203	0.71	0/26228

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	6281	0	6210	83	0
1	D	6276	0	6206	96	0
2	B	2507	0	2473	26	0
2	E	2507	0	2473	27	0
3	C	502	0	545	4	0
3	F	492	0	538	6	0
4	A	85	0	128	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	85	0	128	4	0
5	A	130	0	124	16	0
5	D	130	0	124	20	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	A	40	0	68	1	0
8	A	42	0	64	2	0
9	A	1	0	0	0	0
9	D	1	0	0	0	0
10	B	2	0	0	0	0
10	E	2	0	0	0	0
11	B	43	0	30	2	0
11	E	43	0	30	2	0
12	B	21	0	32	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
13	F	1	0	0	0	0
14	A	157	0	0	4	0
14	B	90	0	0	1	0
14	D	111	0	0	0	0
14	E	34	0	0	0	0
All	All	19587	0	19173	230	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 6.

All (230) 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:77:MET:HB3	5:A:1015:HAS:CAC	1.99	0.93
1:D:77:MET:HB3	5:D:1015:HAS:CAC	2.00	0.91
1:D:367:LEU:CB	5:D:1016:HAS:HMD	2.15	0.77
1:D:70:LEU:HD13	5:D:1015:HAS:HBD1	1.66	0.77
1:A:77:MET:HB3	5:A:1015:HAS:HAC	1.68	0.73
1:D:298:ALA:HA	1:D:301:MET:HE2	1.70	0.72
3:C:3:TYR:HB3	3:C:59:ILE:HD11	1.72	0.71
1:A:298:ALA:HA	1:A:301:MET:HE2	1.72	0.71
1:D:367:LEU:HB2	5:D:1016:HAS:HMD	1.72	0.70
3:F:3:TYR:HB3	3:F:59:ILE:HD11	1.73	0.69
2:B:245:GLN:NE2	1:D:150:GLU:HG3	2.08	0.69
1:D:358:LEU:O	1:D:362:ILE:HG12	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LEU:HB3	5:A:1016:HAS:HMD	1.74	0.68
1:A:367:LEU:CB	5:A:1016:HAS:HMD	2.25	0.67
1:A:338:GLY:HA2	2:B:64:PHE:CE1	2.31	0.66
1:D:277:PHE:CE2	2:E:79:GLY:HA2	2.31	0.65
1:A:358:LEU:O	1:A:362:ILE:HG12	1.96	0.64
2:B:307:PRO:HG2	2:E:304:PRO:HG3	1.80	0.63
2:B:245:GLN:HE22	1:D:150:GLU:HG3	1.63	0.63
1:D:70:LEU:HD21	1:D:448:ARG:HG2	1.81	0.63
1:A:40:ALA:HB1	5:A:1015:HAS:H211	1.81	0.63
1:A:70:LEU:HD21	1:A:448:ARG:HG2	1.82	0.62
1:D:298:ALA:HB3	1:D:314:PHE:CG	2.35	0.62
14:A:2082:HOH:O	2:B:77:ILE:HD11	2.01	0.61
5:D:1016:HAS:H323	2:E:98:LEU:HD11	1.84	0.60
1:A:323:VAL:HB	1:A:324:PRO:HD3	1.84	0.60
2:B:127:TRP:CD1	11:B:587:HEC:HAD1	2.38	0.59
1:D:604:HIS:HB3	1:D:605:PRO:HD2	1.85	0.59
1:A:298:ALA:HB3	1:A:314:PHE:CG	2.38	0.58
2:B:135:LEU:HD13	2:B:224:VAL:HG11	1.84	0.58
2:E:127:TRP:CD1	11:E:587:HEC:HAD1	2.38	0.58
1:A:243:GLN:OE1	1:A:301:MET:HE1	2.04	0.58
2:E:238:ARG:HD2	2:E:238:ARG:O	2.03	0.58
1:A:568:PHE:CZ	4:A:900:5PL:H202	2.39	0.58
1:D:323:VAL:HB	1:D:324:PRO:HD3	1.86	0.57
1:D:783:VAL:HG23	3:F:43:LEU:HD11	1.87	0.57
1:D:55:VAL:HB	1:D:56:PRO:HD2	1.88	0.56
1:D:243:GLN:OE1	1:D:301:MET:HE1	2.06	0.55
1:D:77:MET:HB3	5:D:1015:HAS:HAC	1.85	0.55
1:D:298:ALA:HB3	1:D:314:PHE:CD2	2.42	0.55
1:D:367:LEU:HD13	5:D:1016:HAS:HBD2	1.87	0.55
1:D:227:LEU:C	1:D:227:LEU:HD23	2.32	0.55
1:A:165:PHE:HE1	4:A:900:5PL:HBK2	1.72	0.55
1:D:143:TYR:CG	1:D:144:PRO:HA	2.42	0.54
1:D:250:HIS:HB3	1:D:251:PRO:HD3	1.89	0.54
1:A:227:LEU:C	1:A:227:LEU:HD23	2.33	0.54
1:D:618:TRP:HH2	3:F:27:LEU:HD22	1.73	0.54
1:A:258:LEU:HB2	1:A:259:PRO:HD3	1.89	0.54
1:D:362:ILE:HG23	5:D:1016:HAS:H313	1.90	0.54
1:A:157:LEU:HD22	1:A:216:THR:HG23	1.89	0.54
2:E:135:LEU:HD22	2:E:224:VAL:HG11	1.90	0.53
1:A:537:LYS:HB2	1:A:539:VAL:HG23	1.90	0.53
1:D:367:LEU:C	5:D:1016:HAS:HMD	2.34	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:ILE:HG22	2:B:199:GLU:HG2	1.91	0.52
1:D:258:LEU:HB2	1:D:259:PRO:HD3	1.91	0.52
1:D:783:VAL:HG23	3:F:43:LEU:CD1	2.39	0.52
1:A:49:ILE:CG2	5:A:1015:HAS:HMD	2.40	0.52
1:A:143:TYR:CG	1:A:144:PRO:HA	2.45	0.52
1:D:157:LEU:HD22	1:D:216:THR:HG23	1.92	0.51
1:D:256:MET:O	1:D:260:TYR:HD2	1.93	0.51
2:E:135:LEU:HD13	2:E:224:VAL:HG11	1.93	0.51
2:E:57:LEU:O	2:E:61:THR:HG23	2.10	0.51
1:A:353:PHE:CD1	1:A:353:PHE:C	2.89	0.51
1:A:366:MET:SD	7:A:1200:4AG:H352	2.50	0.51
1:A:250:HIS:HB3	1:A:251:PRO:HD3	1.93	0.50
2:B:57:LEU:O	2:B:61:THR:HG23	2.11	0.50
1:D:679:HIS:CE1	1:D:683:ARG:CZ	2.94	0.50
1:A:298:ALA:HB3	1:A:314:PHE:CD2	2.46	0.50
1:A:55:VAL:HB	1:A:56:PRO:HD2	1.93	0.50
1:A:209:LEU:HA	1:A:248:TYR:CD1	2.46	0.50
1:D:40:ALA:HB1	5:D:1015:HAS:H253	1.93	0.50
1:D:435:LEU:HB2	1:D:436:PRO:HD3	1.93	0.50
1:D:386:PHE:HB2	5:D:1016:HAS:HMA3	1.93	0.50
1:A:106:LEU:HD13	4:A:900:5PL:HBV1	1.93	0.50
2:E:142:GLU:HG2	2:E:211:ARG:HB2	1.94	0.49
1:D:353:PHE:CD1	1:D:353:PHE:C	2.90	0.49
1:A:256:MET:O	1:A:260:TYR:HD2	1.96	0.49
1:A:612:THR:HA	3:C:28:THR:HG22	1.95	0.49
1:D:387:HIS:O	1:D:391:MET:HB3	2.12	0.49
1:A:98:MET:HB3	1:A:192:PRO:HG2	1.95	0.49
1:A:658:TRP:CH2	1:A:659:LEU:HD13	2.46	0.49
1:D:277:PHE:CD2	2:E:79:GLY:HA2	2.48	0.49
1:D:209:LEU:HA	1:D:248:TYR:CD1	2.48	0.49
2:E:161:ILE:HG22	2:E:199:GLU:HG2	1.95	0.49
1:A:677:ALA:HB2	1:A:692:GLY:HA3	1.95	0.48
1:D:298:ALA:CA	1:D:301:MET:HE2	2.42	0.48
1:D:658:TRP:CH2	1:D:659:LEU:HD13	2.48	0.48
1:A:70:LEU:HD13	5:A:1015:HAS:HBD1	1.95	0.48
1:D:607:GLU:O	1:D:607:GLU:HG3	2.13	0.48
2:B:222:ARG:NH1	14:B:2044:HOH:O	2.46	0.48
1:A:435:LEU:HB2	1:A:436:PRO:HD3	1.95	0.48
1:A:49:ILE:HG21	5:A:1015:HAS:HMD	1.95	0.48
1:A:274:LYS:HE2	1:A:335:THR:O	2.14	0.48
1:A:675:HIS:HD2	14:A:2157:HOH:O	1.97	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:HIS:CD2	1:D:250:HIS:C	2.91	0.48
1:D:252:THR:O	1:D:256:MET:HG3	2.13	0.47
1:A:316:PHE:HB2	2:B:99:PHE:CE1	2.49	0.47
2:B:231:PRO:HG3	1:D:715:TYR:OH	2.14	0.47
1:D:367:LEU:HB3	5:D:1016:HAS:HMD	1.95	0.47
2:B:90:ILE:HB	2:B:91:PRO:HD3	1.97	0.47
2:B:142:GLU:HG2	2:B:211:ARG:HB2	1.97	0.47
1:D:386:PHE:HB2	5:D:1016:HAS:CMA	2.45	0.47
1:A:370:THR:HB	1:A:371:PRO:HD3	1.97	0.47
3:C:21:ILE:HG23	3:C:22:LEU:HG	1.97	0.47
1:D:340:LYS:HE2	2:E:72:GLU:O	2.14	0.47
1:D:316:PHE:HB2	2:E:99:PHE:CE1	2.49	0.47
1:A:175:VAL:HG11	1:A:623:TRP:CE2	2.51	0.46
1:D:103:ASP:OD2	1:D:552:PRO:HG2	2.15	0.46
1:D:256:MET:O	1:D:260:TYR:CD2	2.68	0.46
1:D:264:LEU:HD11	1:D:353:PHE:CG	2.51	0.46
1:D:390:LEU:HG	5:D:1016:HAS:HAC	1.97	0.46
1:A:264:LEU:HD11	1:A:353:PHE:CG	2.51	0.46
1:D:370:THR:HB	1:D:371:PRO:HD3	1.97	0.46
2:E:280:VAL:HG13	2:E:286:ASN:ND2	2.30	0.46
1:A:228:SER:HA	14:A:2066:HOH:O	2.16	0.46
1:A:250:HIS:C	1:A:250:HIS:CD2	2.94	0.46
1:A:252:THR:O	1:A:256:MET:HG3	2.16	0.46
2:E:90:ILE:HB	2:E:91:PRO:HD3	1.98	0.46
1:D:321:ILE:O	1:D:324:PRO:HD2	2.16	0.45
1:D:679:HIS:CE1	1:D:683:ARG:NH1	2.84	0.45
1:D:683:ARG:HG2	1:D:685:ARG:HH21	1.81	0.45
1:A:387:HIS:O	1:A:391:MET:HB3	2.16	0.45
1:A:358:LEU:HD21	2:B:53:VAL:HG11	1.97	0.45
1:D:274:LYS:HE2	1:D:335:THR:O	2.16	0.45
2:B:264:PRO:HD2	11:B:587:HEC:C3D	2.46	0.45
1:A:143:TYR:CE1	1:A:144:PRO:HB3	2.52	0.45
1:A:179:TYR:CE2	3:C:27:LEU:HD12	2.51	0.45
1:A:256:MET:O	1:A:260:TYR:CD2	2.70	0.45
1:A:250:HIS:CE1	1:A:254:TYR:OH	2.68	0.45
2:B:125:GLN:HA	2:B:126:PHE:HA	1.76	0.45
2:B:135:LEU:HD22	2:B:224:VAL:HG11	1.98	0.45
1:D:515:HIS:O	1:D:516:ASN:HB2	2.17	0.45
2:E:241:GLN:O	2:E:245:GLN:HG3	2.17	0.45
5:A:1015:HAS:H251	5:A:1015:HAS:H281	1.65	0.45
1:A:250:HIS:O	1:A:253:VAL:HG22	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ALA:CA	1:A:301:MET:HE2	2.43	0.44
1:A:402:LEU:O	1:A:406:TRP:HB2	2.17	0.44
4:D:900:5PL:OCO	4:D:900:5PL:HAY1	2.16	0.44
2:E:294:PRO:HB2	2:E:301:VAL:HG11	1.98	0.44
1:A:416:GLU:O	1:A:420:ARG:HG3	2.18	0.44
1:A:210:ALA:HB1	1:A:631:LEU:HA	2.00	0.44
1:A:422:HIS:CE1	1:A:480:TRP:HB2	2.53	0.44
1:D:659:LEU:HD12	1:D:659:LEU:HA	1.85	0.44
2:E:238:ARG:O	2:E:242:VAL:HG23	2.18	0.44
1:A:689:PHE:CE1	1:A:767:LEU:HD22	2.53	0.44
3:F:21:ILE:HG23	3:F:22:LEU:HG	2.00	0.44
1:A:367:LEU:C	5:A:1016:HAS:HMD	2.42	0.44
1:A:507:LEU:O	1:A:507:LEU:HG	2.17	0.44
1:D:210:ALA:HB1	1:D:631:LEU:HA	2.00	0.44
1:D:383:VAL:HA	1:D:386:PHE:CE2	2.53	0.44
1:A:29:LEU:HD22	8:A:1300:7E8:H42C	2.00	0.43
1:D:43:GLY:HA3	5:D:1015:HAS:H161	2.00	0.43
1:D:194:TYR:HB2	1:D:266:GLU:HG3	1.99	0.43
1:D:367:LEU:HB2	5:D:1016:HAS:CMD	2.45	0.43
1:D:738:LEU:HD11	4:D:900:5PL:H202	2.00	0.43
1:A:604:HIS:HB3	1:A:605:PRO:HD2	1.99	0.43
1:D:422:HIS:CE1	1:D:480:TRP:HB2	2.53	0.43
1:D:250:HIS:CE1	1:D:254:TYR:OH	2.71	0.43
2:E:84:GLU:HA	2:E:87:TRP:NE1	2.33	0.43
2:B:294:PRO:HB2	2:B:301:VAL:HG11	2.00	0.43
1:A:510:SER:HA	1:A:511:PRO:HA	1.88	0.43
1:D:250:HIS:O	1:D:253:VAL:HG22	2.18	0.43
4:A:900:5PL:HAY1	4:A:900:5PL:OCO	2.19	0.43
2:E:165:TRP:CG	2:E:172:LYS:HE3	2.53	0.43
8:A:1301:7E8:H191	14:A:2010:HOH:O	2.18	0.43
1:D:143:TYR:CE1	1:D:144:PRO:HB3	2.53	0.43
1:D:485:TRP:O	1:D:489:ARG:HG2	2.18	0.43
1:A:40:ALA:HB1	5:A:1015:HAS:C21	2.47	0.42
1:A:742:ILE:HG23	4:A:900:5PL:CBR	2.49	0.42
5:A:1015:HAS:HHA	5:A:1015:HAS:HAD2	1.88	0.42
1:A:367:LEU:HD13	5:A:1016:HAS:CBF	2.50	0.42
1:D:98:MET:HB3	1:D:192:PRO:HG2	2.00	0.42
1:D:99:LEU:HD21	1:D:195:VAL:HG11	2.01	0.42
1:D:742:ILE:HG23	4:D:900:5PL:CBR	2.50	0.42
1:D:27:ILE:HD13	1:D:30:MET:CE	2.49	0.42
1:D:175:VAL:HG11	1:D:623:TRP:CE2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:308:GLN:O	2:E:309:LEU:C	2.62	0.42
1:A:634:ILE:HD12	1:A:634:ILE:HA	1.94	0.42
1:D:586:LEU:HD12	1:D:586:LEU:HA	1.93	0.42
2:B:165:TRP:CG	2:B:172:LYS:HE3	2.55	0.42
1:D:402:LEU:O	1:D:406:TRP:HB2	2.19	0.42
1:D:264:LEU:HD11	1:D:353:PHE:CD1	2.55	0.42
1:D:612:THR:HA	3:F:28:THR:HG22	2.01	0.42
2:E:125:GLN:HA	2:E:126:PHE:HA	1.75	0.42
1:A:390:LEU:HD23	5:A:1016:HAS:HBC2	2.02	0.42
1:D:358:LEU:HD21	2:E:53:VAL:HG11	2.02	0.42
1:A:196:TRP:O	1:A:199:PHE:HB3	2.19	0.41
1:A:321:ILE:O	1:A:324:PRO:HD2	2.19	0.41
1:A:515:HIS:O	1:A:516:ASN:HB2	2.19	0.41
2:B:308:GLN:HG3	2:E:302:LYS:HA	2.01	0.41
1:D:751:TYR:CE2	1:D:755:LEU:HD11	2.55	0.41
1:A:622:ALA:HB2	1:A:772:MET:HE1	2.03	0.41
1:A:680:ASP:OD2	1:A:688:PRO:HB2	2.19	0.41
1:D:218:LEU:HD21	1:D:731:THR:HG21	2.03	0.41
1:D:241:PHE:CD1	1:D:241:PHE:C	2.98	0.41
1:D:260:TYR:O	1:D:264:LEU:HG	2.21	0.41
1:A:354:ILE:CG2	2:B:57:LEU:HD22	2.51	0.41
1:A:361:GLY:HA3	5:A:1016:HAS:C15	2.51	0.41
1:D:687:ASN:HB2	1:D:688:PRO:HD3	2.03	0.41
4:D:900:5PL:OCO	4:D:900:5PL:HBH	2.19	0.41
1:A:27:ILE:HD13	1:A:30:MET:CE	2.50	0.41
1:D:43:GLY:HA3	5:D:1015:HAS:C16	2.51	0.41
1:D:386:PHE:CD2	5:D:1016:HAS:HAA1	2.56	0.41
1:A:264:LEU:HD11	1:A:353:PHE:CD1	2.55	0.41
2:B:223:PHE:HA	2:B:329:PHE:CZ	2.55	0.41
1:D:274:LYS:NZ	1:D:337:TRP:O	2.51	0.41
1:D:406:TRP:HB3	1:D:407:PRO:HD3	2.01	0.41
2:E:275:LEU:HD12	11:E:587:HEC:HAA1	2.02	0.41
1:A:99:LEU:HD21	1:A:195:VAL:HG11	2.03	0.41
1:A:751:TYR:CE2	1:A:755:LEU:HD11	2.55	0.41
1:D:507:LEU:HG	1:D:507:LEU:O	2.21	0.41
2:E:232:ALA:HA	2:E:233:PRO:HD3	1.95	0.41
1:A:68:GLN:HG3	1:A:136:SER:HB3	2.03	0.41
1:A:367:LEU:HD21	1:A:381:PHE:HD1	1.86	0.41
2:B:232:ALA:HA	2:B:233:PRO:HD3	1.94	0.41
1:A:367:LEU:CB	5:A:1016:HAS:CMD	2.98	0.41
1:D:196:TRP:O	1:D:199:PHE:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:TYR:HB2	1:A:266:GLU:HG3	2.03	0.40
2:B:69:GLU:O	2:B:71:GLN:HG2	2.21	0.40
1:D:114:TYR:O	1:D:117:PHE:HB3	2.20	0.40
1:D:510:SER:HA	1:D:511:PRO:HA	1.88	0.40
2:E:158:LYS:HA	2:E:158:LYS:HD3	1.92	0.40
1:D:459:TRP:HB2	1:D:460:PRO:HD3	2.02	0.40
5:D:1015:HAS:H281	5:D:1015:HAS:H251	1.35	0.40
1:A:231:ASN:HA	1:A:232:PRO:HD3	1.92	0.40
1:D:363:THR:HG21	1:D:438:TYR:CE1	2.56	0.40
5:D:1016:HAS:HMC1	5:D:1016:HAS:HBC1	2.04	0.40
2:B:280:VAL:HG13	2:B:286:ASN:ND2	2.36	0.40
1:D:465:LEU:HD23	1:D:465:LEU:HA	1.95	0.40
1:D:649:THR:HA	1:D:650:PRO:HD3	1.96	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	779/791 (98%)	762 (98%)	17 (2%)	0	100	100
1	D	778/791 (98%)	759 (98%)	19 (2%)	0	100	100
2	B	317/337 (94%)	308 (97%)	9 (3%)	0	100	100
2	E	317/337 (94%)	307 (97%)	10 (3%)	0	100	100
3	C	62/66 (94%)	62 (100%)	0	0	100	100
3	F	61/66 (92%)	61 (100%)	0	0	100	100
All	All	2314/2388 (97%)	2259 (98%)	55 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	640/646 (99%)	637 (100%)	3 (0%)	81	89
1	D	639/646 (99%)	635 (99%)	4 (1%)	78	87
2	B	261/274 (95%)	257 (98%)	4 (2%)	57	72
2	E	261/274 (95%)	256 (98%)	5 (2%)	50	65
3	C	51/53 (96%)	50 (98%)	1 (2%)	48	63
3	F	50/53 (94%)	50 (100%)	0	100	100
All	All	1902/1946 (98%)	1885 (99%)	17 (1%)	70	82

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	378	ASP
1	A	432	LEU
1	A	759	ILE
2	B	194	TYR
2	B	272	ARG
2	B	275	LEU
2	B	280	VAL
3	C	64	HIS
1	D	321	ILE
1	D	378	ASP
1	D	432	LEU
1	D	595	ARG
2	E	50	PHE
2	E	194	TYR
2	E	238	ARG
2	E	272	ARG
2	E	280	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	550	HIS
1	A	675	HIS
2	B	26	HIS
2	B	71	GLN
2	B	78	HIS
2	B	241	GLN
2	B	245	GLN
3	C	63	HIS
1	D	57	ASN
1	D	171	ASN
1	D	205	ASN
1	D	550	HIS
1	D	679	HIS
1	D	764	HIS
2	E	26	HIS
2	E	244	GLN
3	F	63	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
3	FME	F	1	3	8,9,10	0.38	0	7,9,11	0.69	0
3	FME	C	1	3	8,9,10	0.36	0	7,9,11	1.31	1 (14%)

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
3	FME	F	1	3	-	0/7/9/11	-
3	FME	C	1	3	-	0/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	CA-N-CN	-2.92	118.33	122.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 7 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	HAS	D	1015	1	71,72,72	2.04	18 (25%)	84,109,109	2.39	29 (34%)
11	HEC	E	587	2	50,50,50	1.75	5 (10%)	68,82,82	1.62	7 (10%)
8	7E8	A	1300	-	20,20,20	1.05	1 (5%)	21,21,21	0.96	1 (4%)
8	7E8	A	1301	-	20,20,20	1.01	1 (5%)	21,21,21	1.04	2 (9%)
10	CUA	E	585	2	0,1,1	-	-	-	-	-
7	4AG	A	1200	-	39,39,39	1.06	2 (5%)	41,41,41	1.21	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CUA	B	585	2	0,1,1	-	-	-		
4	5PL	A	900	-	84,85,85	0.81	2 (2%)	96,101,101	1.02	4 (4%)
5	HAS	D	1016	14,1	71,72,72	1.86	16 (22%)	84,109,109	2.46	29 (34%)
11	HEC	B	587	2	50,50,50	1.59	6 (12%)	68,82,82	1.51	7 (10%)
4	5PL	D	900	-	84,85,85	0.81	2 (2%)	96,101,101	1.09	9 (9%)
5	HAS	A	1016	14,1	71,72,72	2.02	15 (21%)	84,109,109	2.40	28 (33%)
12	7E9	B	701	-	20,20,20	1.06	1 (5%)	21,21,21	1.20	1 (4%)
5	HAS	A	1015	1	71,72,72	1.88	15 (21%)	84,109,109	2.38	33 (39%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HAS	D	1015	1	1/1/8/18	11/42/82/82	-
11	HEC	E	587	2	1/1/3/7	4/14/54/54	-
8	7E8	A	1300	-	1/1/2/4	6/20/20/20	-
8	7E8	A	1301	-	-	6/20/20/20	-
7	4AG	A	1200	-	-	15/41/41/41	-
11	HEC	B	587	2	1/1/3/7	5/14/54/54	-
5	HAS	D	1016	14,1	1/1/8/18	10/42/82/82	-
4	5PL	A	900	-	-	30/87/107/107	0/1/1/1
12	7E9	B	701	-	-	7/21/21/21	-
4	5PL	D	900	-	-	26/87/107/107	0/1/1/1
5	HAS	A	1016	14,1	1/1/8/18	9/42/82/82	-
5	HAS	A	1015	1	1/1/8/18	13/42/82/82	-

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	E	587	HEC	C3D-C2D	7.70	1.53	1.36
5	D	1015	HAS	FE-NB	7.70	2.18	1.94
5	A	1015	HAS	FE-NB	7.54	2.18	1.94
11	B	587	HEC	C3D-C2D	7.30	1.52	1.36
5	A	1016	HAS	FE-NB	6.95	2.16	1.94
5	D	1016	HAS	FE-NB	6.41	2.14	1.94
5	D	1015	HAS	FE-ND	5.88	2.13	1.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1016	HAS	FE-NC	5.76	2.14	1.95
5	A	1016	HAS	FE-ND	5.35	2.11	1.94
5	D	1015	HAS	FE-NA	5.03	2.12	1.95
5	A	1015	HAS	FE-NA	4.89	2.11	1.95
5	D	1015	HAS	C3B-C2B	4.88	1.45	1.34
5	D	1015	HAS	C2D-C3D	4.80	1.47	1.36
5	D	1016	HAS	C3B-C2B	4.75	1.45	1.34
5	A	1016	HAS	C2D-C3D	4.75	1.46	1.36
5	A	1015	HAS	C2A-C3A	4.74	1.46	1.36
5	D	1016	HAS	C2A-C3A	4.73	1.46	1.36
5	D	1016	HAS	FE-NA	4.72	2.11	1.95
5	A	1016	HAS	C2A-C3A	4.71	1.46	1.36
5	A	1016	HAS	FE-NA	4.69	2.11	1.95
5	A	1016	HAS	C3B-C2B	4.67	1.45	1.34
4	D	900	5PL	OCK-CBU	4.66	1.47	1.34
7	A	1200	4AG	O17-C16	4.52	1.46	1.33
5	A	1015	HAS	C3B-C2B	4.45	1.44	1.34
8	A	1300	7E8	O16-C8	4.44	1.46	1.33
4	A	900	5PL	OCL-CBL	4.41	1.46	1.33
5	D	1016	HAS	FE-ND	4.41	2.08	1.94
4	A	900	5PL	OCK-CBU	4.41	1.46	1.34
5	D	1015	HAS	C2A-C3A	4.36	1.46	1.36
5	D	1016	HAS	C2D-C3D	4.27	1.45	1.36
11	E	587	HEC	FE-NB	4.26	2.08	1.94
8	A	1301	7E8	O16-C8	4.26	1.45	1.33
12	B	701	7E9	O1-C80	4.26	1.46	1.34
5	A	1015	HAS	C2D-C3D	4.25	1.45	1.36
7	A	1200	4AG	O21-C22	4.24	1.46	1.34
5	D	1015	HAS	FE-NC	4.18	2.09	1.95
4	D	900	5PL	OCL-CBL	3.93	1.44	1.33
11	E	587	HEC	FE-ND	3.75	2.06	1.94
11	E	587	HEC	FE-NA	3.62	2.07	1.95
5	A	1016	HAS	C4B-C3B	3.57	1.50	1.44
5	D	1016	HAS	C4B-C3B	3.47	1.50	1.44
5	A	1016	HAS	C1B-C2B	3.42	1.51	1.44
5	D	1016	HAS	FE-NC	3.38	2.06	1.95
5	A	1015	HAS	C4B-C3B	3.35	1.50	1.44
5	A	1015	HAS	FE-NC	3.33	2.06	1.95
5	A	1015	HAS	FE-ND	3.31	2.05	1.94
5	D	1015	HAS	C4B-C3B	3.21	1.50	1.44
11	B	587	HEC	FE-NB	3.04	2.04	1.94
5	D	1016	HAS	C4D-C3D	2.93	1.50	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	587	HEC	FE-ND	2.79	2.03	1.94
5	D	1015	HAS	C4D-C3D	2.76	1.49	1.45
5	A	1016	HAS	C1C-C2C	2.73	1.49	1.43
5	A	1016	HAS	C1D-ND	-2.70	1.35	1.40
5	A	1015	HAS	C1D-ND	-2.67	1.35	1.40
5	D	1016	HAS	C1D-ND	-2.66	1.35	1.40
5	D	1015	HAS	C1D-ND	-2.57	1.35	1.40
5	A	1015	HAS	C1B-C2B	2.56	1.49	1.44
5	D	1016	HAS	C1A-C2A	2.55	1.49	1.45
5	A	1015	HAS	C1C-C2C	2.54	1.49	1.43
5	A	1015	HAS	C4B-NB	-2.47	1.36	1.40
5	D	1015	HAS	C3C-C4C	2.39	1.48	1.42
5	A	1015	HAS	C4A-NA	-2.39	1.35	1.39
5	D	1015	HAS	C1C-C2C	2.39	1.48	1.43
5	A	1016	HAS	C3C-C4C	2.38	1.48	1.42
5	A	1015	HAS	C1A-NA	-2.32	1.35	1.39
5	D	1015	HAS	C4B-NB	-2.29	1.36	1.40
11	B	587	HEC	FE-NC	2.26	2.02	1.95
5	D	1016	HAS	C4A-NA	-2.26	1.35	1.39
5	A	1016	HAS	C4A-C3A	2.25	1.49	1.45
5	D	1016	HAS	C1C-C2C	2.22	1.48	1.43
5	D	1015	HAS	C4A-C3A	2.21	1.49	1.45
5	D	1016	HAS	C3C-C4C	2.21	1.47	1.42
5	D	1015	HAS	C1A-NA	-2.18	1.35	1.39
5	D	1015	HAS	C4A-NA	-2.17	1.35	1.39
5	D	1015	HAS	C1B-C2B	2.15	1.48	1.44
5	A	1016	HAS	C1A-C2A	2.12	1.49	1.45
11	B	587	HEC	FE-NA	2.12	2.02	1.95
11	E	587	HEC	FE-NC	2.11	2.02	1.95
5	A	1015	HAS	C3C-C4C	2.09	1.47	1.42
11	B	587	HEC	CMB-C2B	2.08	1.55	1.50
5	D	1016	HAS	C4A-C3A	2.05	1.49	1.45
5	D	1016	HAS	C4B-NB	-2.04	1.36	1.40
5	A	1016	HAS	C4D-C3D	2.03	1.48	1.45
5	D	1015	HAS	C1A-C2A	2.01	1.48	1.45

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1016	HAS	C2D-C3D-C4D	-7.99	100.79	106.49
5	D	1016	HAS	C2D-C3D-C4D	-7.96	100.82	106.49
5	A	1015	HAS	C2D-C3D-C4D	-7.92	100.84	106.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1016	HAS	CAD-CBD-CGD	-7.68	97.07	113.60
5	D	1015	HAS	C2D-C3D-C4D	-7.12	101.41	106.49
5	D	1015	HAS	C4C-NC-C1C	6.76	111.97	105.35
5	D	1016	HAS	CAD-CBD-CGD	-6.58	99.43	113.60
11	E	587	HEC	C1D-ND-C4D	6.36	111.64	105.07
5	A	1015	HAS	C4C-NC-C1C	6.21	111.43	105.35
5	D	1016	HAS	C4C-NC-C1C	5.70	110.93	105.35
5	A	1016	HAS	C4C-NC-C1C	5.69	110.92	105.35
5	D	1015	HAS	C4B-NB-C1B	5.68	110.94	105.07
5	D	1015	HAS	CAD-CBD-CGD	-5.61	101.53	113.60
11	B	587	HEC	C1D-ND-C4D	5.40	110.65	105.07
5	A	1016	HAS	C1D-ND-C4D	5.39	110.64	105.07
5	A	1016	HAS	CAA-CBA-CGA	-5.37	102.04	113.60
5	A	1015	HAS	C4B-NB-C1B	5.29	110.53	105.07
5	D	1015	HAS	C1D-ND-C4D	5.25	110.49	105.07
5	D	1015	HAS	C4A-NA-C1A	5.20	110.44	105.35
5	A	1015	HAS	CAD-CBD-CGD	-5.11	102.60	113.60
11	B	587	HEC	CBD-CAD-C3D	-5.10	98.45	112.63
5	D	1016	HAS	C13-C12-C11	-5.03	106.78	114.35
11	E	587	HEC	CBD-CAD-C3D	-5.02	98.69	112.63
5	A	1015	HAS	C1D-ND-C4D	4.62	109.84	105.07
5	D	1016	HAS	C4B-NB-C1B	4.50	109.72	105.07
5	D	1015	HAS	C3C-C4C-NC	-4.35	107.57	110.25
5	A	1015	HAS	CHA-C4D-C3D	-4.31	118.50	124.84
4	D	900	5PL	OCK-CBU-CBV	4.31	120.78	111.50
5	D	1016	HAS	CMC-C2C-C1C	-4.30	118.82	125.37
4	A	900	5PL	OCK-CBU-CBV	4.21	120.58	111.50
5	A	1015	HAS	OMD-CMD-C2D	-4.19	116.20	125.69
5	D	1016	HAS	CHB-C1D-ND	4.18	129.52	124.37
5	A	1016	HAS	C4B-NB-C1B	4.17	109.38	105.07
7	A	1200	4AG	O21-C22-C23	4.12	120.37	111.50
5	D	1016	HAS	CAA-CBA-CGA	-4.09	104.80	113.60
5	A	1016	HAS	CMC-C2C-C1C	-4.08	119.16	125.37
5	A	1016	HAS	C13-C12-C11	-4.08	108.23	114.35
12	B	701	7E9	O1-C80-C2	4.04	120.20	111.50
5	D	1016	HAS	CMC-C2C-C3C	4.03	136.34	126.59
5	D	1016	HAS	CMA-C3A-C4A	-4.01	117.65	124.71
5	D	1015	HAS	C13-C12-C11	-4.00	108.33	114.35
5	A	1016	HAS	CMC-C2C-C3C	3.98	136.22	126.59
5	D	1016	HAS	C1D-ND-C4D	3.98	109.18	105.07
5	A	1015	HAS	CHA-C4D-ND	3.96	128.72	124.42
5	D	1016	HAS	CAD-C3D-C4D	3.92	131.51	124.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1016	HAS	C13-C14-C15	-3.83	118.43	127.66
5	D	1015	HAS	CMC-C2C-C3C	3.80	135.80	126.59
5	D	1016	HAS	C1A-C2A-C3A	-3.80	102.17	107.13
5	A	1015	HAS	C4A-NA-C1A	3.80	109.07	105.35
5	A	1016	HAS	C4A-NA-C1A	3.78	109.05	105.35
5	D	1015	HAS	CMC-C2C-C1C	-3.76	119.64	125.37
5	A	1015	HAS	C3C-C4C-NC	-3.68	107.98	110.25
5	A	1015	HAS	C1A-C2A-C3A	-3.64	102.38	107.13
5	D	1016	HAS	C4A-NA-C1A	3.60	108.87	105.35
5	A	1016	HAS	C1A-C2A-C3A	-3.50	102.56	107.13
5	D	1016	HAS	CMA-C3A-C2A	3.47	135.54	126.12
5	A	1015	HAS	CMC-C2C-C3C	3.46	134.98	126.59
5	D	1016	HAS	CMB-C2B-C1B	-3.45	119.79	125.04
5	D	1015	HAS	CBA-CAA-C2A	-3.42	103.11	112.63
5	D	1015	HAS	CMB-C2B-C1B	-3.42	119.83	125.04
5	D	1015	HAS	C21-C22-C23	-3.35	119.59	127.66
5	A	1016	HAS	OMD-CMD-C2D	-3.35	118.12	125.69
5	D	1015	HAS	C13-C14-C15	-3.33	119.65	127.66
4	D	900	5PL	CBH-OCK-CBU	-3.32	109.61	117.79
5	A	1016	HAS	C13-C14-C15	-3.30	119.72	127.66
8	A	1301	7E8	O16-C8-C7	3.22	122.02	111.91
5	A	1015	HAS	C26-C15-C16	3.20	120.66	115.27
4	A	900	5PL	CBH-OCK-CBU	-3.10	110.15	117.79
5	A	1016	HAS	CMA-C3A-C4A	-3.08	119.28	124.71
5	A	1015	HAS	CMA-C3A-C2A	3.07	134.46	126.12
5	A	1015	HAS	C13-C12-C11	-3.03	109.80	114.35
5	A	1015	HAS	CMA-C3A-C4A	-3.02	119.39	124.71
5	A	1015	HAS	C1D-C2D-C3D	3.02	109.51	107.11
5	A	1015	HAS	CMC-C2C-C1C	-2.92	120.92	125.37
5	D	1015	HAS	C1A-C2A-C3A	-2.92	103.32	107.13
5	A	1015	HAS	C25-C23-C24	2.89	120.13	115.27
4	A	900	5PL	CAY-CAX-NCB	-2.88	103.97	112.21
5	A	1016	HAS	CMA-C3A-C2A	2.88	133.93	126.12
5	D	1016	HAS	C27-C19-C20	2.86	120.09	115.27
4	D	900	5PL	C3-C2-N2	-2.86	105.21	110.62
5	A	1015	HAS	CHB-C1D-ND	2.84	127.88	124.37
5	D	1016	HAS	C26-C15-C16	2.84	120.05	115.27
11	E	587	HEC	C4B-NB-C1B	2.79	107.96	105.07
5	A	1016	HAS	C21-C22-C23	-2.79	120.95	127.66
5	D	1016	HAS	OMD-CMD-C2D	-2.78	119.40	125.69
5	D	1015	HAS	C17-C18-C19	-2.77	121.00	127.66
4	D	900	5PL	OCL-CBL-CBM	2.76	120.58	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	587	HEC	CHA-C4D-ND	2.76	127.42	124.42
5	D	1016	HAS	C3C-C4C-NC	-2.76	108.55	110.25
5	D	1015	HAS	OMD-CMD-C2D	-2.75	119.46	125.69
5	D	1015	HAS	C27-C19-C20	2.72	119.86	115.27
5	A	1015	HAS	CHD-C4C-NC	2.72	128.86	123.85
7	A	1200	4AG	O17-C16-C15	2.71	120.42	111.91
5	A	1016	HAS	C1D-C2D-C3D	2.71	109.27	107.11
5	D	1015	HAS	C25-C23-C24	2.70	119.82	115.27
5	A	1015	HAS	CBA-CAA-C2A	-2.70	105.12	112.63
11	E	587	HEC	CBA-CAA-C2A	-2.67	105.20	112.63
5	A	1016	HAS	C27-C19-C20	2.65	119.73	115.27
5	D	1016	HAS	C21-C22-C23	-2.64	121.31	127.66
8	A	1300	7E8	O16-C8-C7	2.63	120.18	111.91
11	B	587	HEC	CBC-CAC-C3C	2.63	119.67	112.43
5	D	1016	HAS	CMB-C2B-C3B	2.61	135.31	130.34
4	A	900	5PL	OCL-CBL-CBM	2.55	119.91	111.91
5	A	1015	HAS	C17-C18-C19	-2.54	121.53	127.66
5	A	1015	HAS	C3C-C2C-C1C	-2.54	104.10	107.16
5	A	1016	HAS	CHB-C1D-ND	2.54	127.50	124.37
5	D	1015	HAS	C32-C30-C31	2.53	120.19	114.60
5	A	1015	HAS	C3D-C4D-ND	2.49	112.77	110.36
5	D	1015	HAS	C26-C15-C16	2.49	119.45	115.27
4	D	900	5PL	OCG-CAN-CAM	2.46	110.61	106.56
5	D	1016	HAS	C1D-C2D-C3D	2.41	109.03	107.11
5	D	1015	HAS	CMA-C3A-C2A	2.40	132.63	126.12
5	A	1016	HAS	C32-C30-C31	2.39	119.88	114.60
11	B	587	HEC	CMD-C2D-C1D	2.39	128.68	125.04
5	A	1015	HAS	C21-C22-C23	-2.39	121.91	127.66
8	A	1301	7E8	O16-C8-O15	-2.38	117.58	123.59
5	D	1016	HAS	CHC-C1C-NC	2.38	128.23	123.85
5	D	1016	HAS	C32-C30-C31	2.38	119.86	114.60
11	E	587	HEC	C4A-NA-C1A	2.38	107.68	105.35
5	D	1016	HAS	C17-C18-C19	-2.37	121.95	127.66
11	E	587	HEC	C3C-C4C-NC	-2.37	107.50	110.15
5	A	1015	HAS	C2A-C1A-NA	2.37	112.63	110.32
5	A	1016	HAS	C17-C18-C19	-2.37	121.96	127.66
7	A	1200	4AG	C6-O21-C22	-2.33	112.06	117.79
5	A	1015	HAS	O2D-CGD-CBD	2.33	121.51	114.03
5	A	1015	HAS	O1D-CGD-CBD	-2.32	115.64	123.08
5	A	1015	HAS	C13-C14-C15	-2.29	122.14	127.66
5	D	1015	HAS	CAA-C2A-C1A	2.28	129.19	124.89
11	B	587	HEC	O2A-CGA-CBA	2.28	121.35	114.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1015	HAS	CMB-C2B-C3B	2.27	134.67	130.34
5	D	1015	HAS	CHB-C1D-ND	2.27	127.17	124.37
11	E	587	HEC	C4C-NC-C1C	2.26	107.56	105.35
5	D	1015	HAS	C28-C29-C30	-2.26	120.02	127.75
5	A	1016	HAS	C3C-C4C-NC	-2.26	108.86	110.25
5	A	1016	HAS	CHA-C1A-C2A	-2.26	121.28	124.94
4	D	900	5PL	O5-C5-C4	2.25	113.78	109.69
5	A	1016	HAS	O1A-CGA-CBA	-2.25	115.86	123.08
5	D	1016	HAS	CHA-C1A-C2A	-2.21	121.35	124.94
5	D	1016	HAS	C25-C23-C24	2.21	118.99	115.27
5	A	1016	HAS	CAD-C3D-C4D	2.19	128.49	124.66
5	A	1016	HAS	C26-C15-C16	2.18	118.94	115.27
4	D	900	5PL	C1-C2-N2	-2.16	107.28	111.00
5	D	1015	HAS	CHD-C4C-NC	2.16	127.83	123.85
5	D	1015	HAS	C3C-C2C-C1C	-2.16	104.55	107.16
11	B	587	HEC	CMC-C2C-C1C	-2.15	122.09	125.37
5	D	1015	HAS	CMA-C3A-C4A	-2.14	120.95	124.71
5	A	1015	HAS	CMB-C2B-C1B	-2.13	121.79	125.04
5	A	1016	HAS	C25-C23-C24	2.13	118.85	115.27
4	D	900	5PL	CAX-NCB-CAP	2.12	126.38	122.59
5	A	1016	HAS	C3C-C2C-C1C	-2.11	104.62	107.16
5	A	1015	HAS	CAA-CBA-CGA	-2.09	109.09	113.60
4	D	900	5PL	C6-C5-C4	-2.03	108.25	113.00
5	A	1015	HAS	C32-C30-C31	2.01	119.05	114.60

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1015	HAS	NA
5	A	1016	HAS	NA
5	D	1015	HAS	NA
5	D	1016	HAS	NA
8	A	1300	7E8	C18
11	B	587	HEC	NA
11	E	587	HEC	NA

All (142) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	900	5PL	CBV-CBU-OCK-CBH
4	D	900	5PL	CBV-CBU-OCK-CBH
5	A	1015	HAS	C1D-C2D-CMD-OMD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1015	HAS	C3D-C2D-CMD-OMD
5	A	1015	HAS	C2D-C3D-CAD-CBD
5	A	1015	HAS	C4D-C3D-CAD-CBD
5	A	1015	HAS	C19-C20-C21-C22
5	A	1016	HAS	C1D-C2D-CMD-OMD
5	A	1016	HAS	C3D-C2D-CMD-OMD
5	D	1015	HAS	C1D-C2D-CMD-OMD
5	D	1015	HAS	C3D-C2D-CMD-OMD
5	D	1015	HAS	C23-C24-C28-C29
5	D	1016	HAS	C1D-C2D-CMD-OMD
5	D	1016	HAS	C3D-C2D-CMD-OMD
12	B	701	7E9	C17-C15-C20-O21
12	B	701	7E9	O1-C15-C20-O21
8	A	1300	7E8	O15-C8-O16-C17
8	A	1300	7E8	C7-C8-O16-C17
4	A	900	5PL	OCN-CBU-OCK-CBH
4	D	900	5PL	OCN-CBU-OCK-CBH
4	D	900	5PL	CBH-CBI-OCL-CBL
4	A	900	5PL	O5-C5-C6-O6
5	A	1015	HAS	C25-C23-C24-C28
5	D	1015	HAS	C25-C23-C24-C28
5	A	1015	HAS	C22-C23-C24-C28
5	D	1015	HAS	C22-C23-C24-C28
4	D	900	5PL	C4-C5-C6-O6
4	A	900	5PL	C4-C5-C6-O6
4	D	900	5PL	CBL-CBM-CBN-CBO
12	B	701	7E9	C80-C2-C3-C4
8	A	1300	7E8	O16-C17-C18-O20
8	A	1300	7E8	O16-C17-C18-C19
4	A	900	5PL	CBJ-C18-C19-C20
7	A	1200	4AG	C26-C27-C28-C29
4	D	900	5PL	CBB-CBC-CBD-CBE
4	D	900	5PL	CBN-CBO-CBP-CAA
4	D	900	5PL	CBR-CBS-CBT-CAL
7	A	1200	4AG	C23-C24-C25-C26
4	D	900	5PL	CBX-CBY-CBZ-CAE
8	A	1301	7E8	C4-C5-C6-C7
4	D	900	5PL	O5-C5-C6-O6
4	A	900	5PL	C19-C18-CBJ-CAV
4	A	900	5PL	CBT-CAL-CAO-CAS
4	D	900	5PL	CAL-CAO-CAS-C7
4	D	900	5PL	CBC-CBD-CBE-CBF

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	900	5PL	CAL-CAO-CAS-C7
8	A	1301	7E8	C3-C4-C5-C6
4	A	900	5PL	CAT-CAU-CAV-CBJ
4	A	900	5PL	C13-C14-C15-C17
4	D	900	5PL	CBJ-C18-C19-C20
4	A	900	5PL	CBX-CBY-CBZ-CAE
4	A	900	5PL	C7-C8-C9-C10
4	D	900	5PL	C19-C18-CBJ-CAV
7	A	1200	4AG	C24-C25-C26-C27
5	A	1015	HAS	C27-C19-C20-C21
4	D	900	5PL	CBW-CBX-CBY-CBZ
4	D	900	5PL	CAF-CAE-CBZ-CBY
8	A	1301	7E8	C11-C10-C9-C1
5	A	1015	HAS	C18-C19-C20-C21
11	B	587	HEC	C2B-C3B-CAB-CBB
4	D	900	5PL	CBT-CAL-CAO-CAS
4	D	900	5PL	CAW-CBH-CBI-OCL
4	A	900	5PL	CAN-CAM-O1-C1
7	A	1200	4AG	C33-C34-C35-C36
8	A	1301	7E8	C7-C8-O16-C17
4	D	900	5PL	C18-C19-C20-C21
12	B	701	7E9	C4-C5-C6-C7
4	D	900	5PL	C14-C13-CBQ-CBK
4	A	900	5PL	CAU-CAT-CBG-CBF
8	A	1300	7E8	C4-C5-C6-C7
4	A	900	5PL	CBU-CBV-CBW-CBX
4	A	900	5PL	CBR-CBS-CBT-CAL
4	A	900	5PL	C14-C13-CBQ-CBK
8	A	1301	7E8	O15-C8-O16-C17
4	A	900	5PL	C7-C8-C9-C12
4	A	900	5PL	CBA-CBB-CBC-CBD
4	A	900	5PL	CBG-CAT-CAU-CAV
4	A	900	5PL	C13-C14-C15-C16
4	D	900	5PL	CAN-OCG-PCR-OCJ
4	A	900	5PL	CAF-CAE-CBZ-CBY
5	D	1016	HAS	C23-C24-C28-C29
4	A	900	5PL	CBB-CBC-CBD-CBE
4	D	900	5PL	OCK-CBH-CBI-OCL
7	A	1200	4AG	C28-C29-C30-C31
11	E	587	HEC	C2C-C3C-CAC-CBC
4	A	900	5PL	CAY-CAZ-CBA-CBB
4	D	900	5PL	CAT-CAU-CAV-CBJ

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	900	5PL	CAE-CAF-CAG-CAK
5	D	1016	HAS	C2D-C3D-CAD-CBD
7	A	1200	4AG	C27-C28-C29-C30
7	A	1200	4AG	C05-C06-C07-C08
5	D	1016	HAS	C4D-C3D-CAD-CBD
4	A	900	5PL	CAE-CAF-CAG-CAK
7	A	1200	4AG	C11-C12-C13-C14
11	B	587	HEC	C4B-C3B-CAB-CBB
7	A	1200	4AG	C13-C14-C15-C16
7	A	1200	4AG	C34-C35-C36-C37
5	D	1015	HAS	C4D-C3D-CAD-CBD
7	A	1200	4AG	O38-C22-O21-C6
12	B	701	7E9	C3-C4-C5-C6
5	A	1015	HAS	CAA-CBA-CGA-O1A
11	B	587	HEC	CAD-CBD-CGD-O1D
11	E	587	HEC	CAD-CBD-CGD-O1D
5	D	1016	HAS	CAA-CBA-CGA-O2A
5	D	1016	HAS	CAD-CBD-CGD-O2D
4	A	900	5PL	CBW-CBX-CBY-CBZ
5	A	1016	HAS	C3A-C2A-CAA-CBA
5	A	1016	HAS	CAA-CBA-CGA-O2A
11	E	587	HEC	CAD-CBD-CGD-O2D
5	A	1016	HAS	CAD-CBD-CGD-O2D
4	A	900	5PL	CAG-CAK-CBK-CBQ
5	A	1016	HAS	CAD-CBD-CGD-O1D
11	B	587	HEC	CAD-CBD-CGD-O2D
5	A	1016	HAS	CAA-CBA-CGA-O1A
5	D	1016	HAS	CAD-CBD-CGD-O1D
5	D	1015	HAS	C27-C19-C20-C21
5	D	1016	HAS	CAA-CBA-CGA-O1A
4	A	900	5PL	C19-C20-C21-C22
5	A	1015	HAS	CAA-CBA-CGA-O2A
5	A	1015	HAS	CAD-CBD-CGD-O2D
11	B	587	HEC	C2C-C3C-CAC-CBC
7	A	1200	4AG	C10-C11-C12-C13
8	A	1301	7E8	C2-C1-C9-C10
5	D	1015	HAS	CAA-CBA-CGA-O1A
5	D	1015	HAS	C2D-C3D-CAD-CBD
4	A	900	5PL	CBP-CAA-CBR-CBS
4	A	900	5PL	CBN-CBO-CBP-CAA
4	D	900	5PL	C19-C20-C21-C22
12	B	701	7E9	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

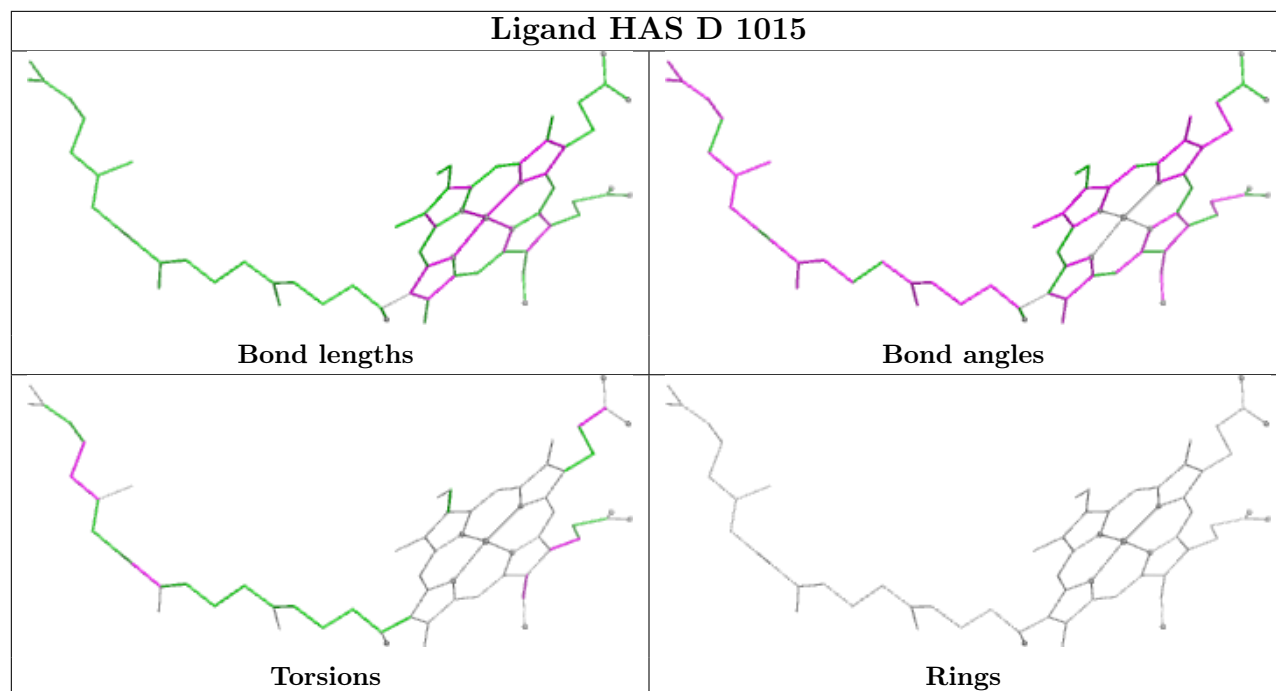
Mol	Chain	Res	Type	Atoms
7	A	1200	4AG	C14-C15-C16-O17
5	D	1015	HAS	CAA-CBA-CGA-O2A
5	A	1015	HAS	CAD-CBD-CGD-O1D
12	B	701	7E9	C7-C8-C9-C10
11	E	587	HEC	C2B-C3B-CAB-CBB
7	A	1200	4AG	C23-C22-O21-C6
5	A	1016	HAS	C1A-C2A-CAA-CBA
8	A	1300	7E8	C6-C7-C8-O16
7	A	1200	4AG	C14-C15-C16-O39
5	A	1016	HAS	C3B-C11-C12-C13
5	D	1016	HAS	C3B-C11-C12-C13
5	D	1015	HAS	C18-C19-C20-C21
4	D	900	5PL	CBR-CAA-CBP-CBO

There are no ring outliers.

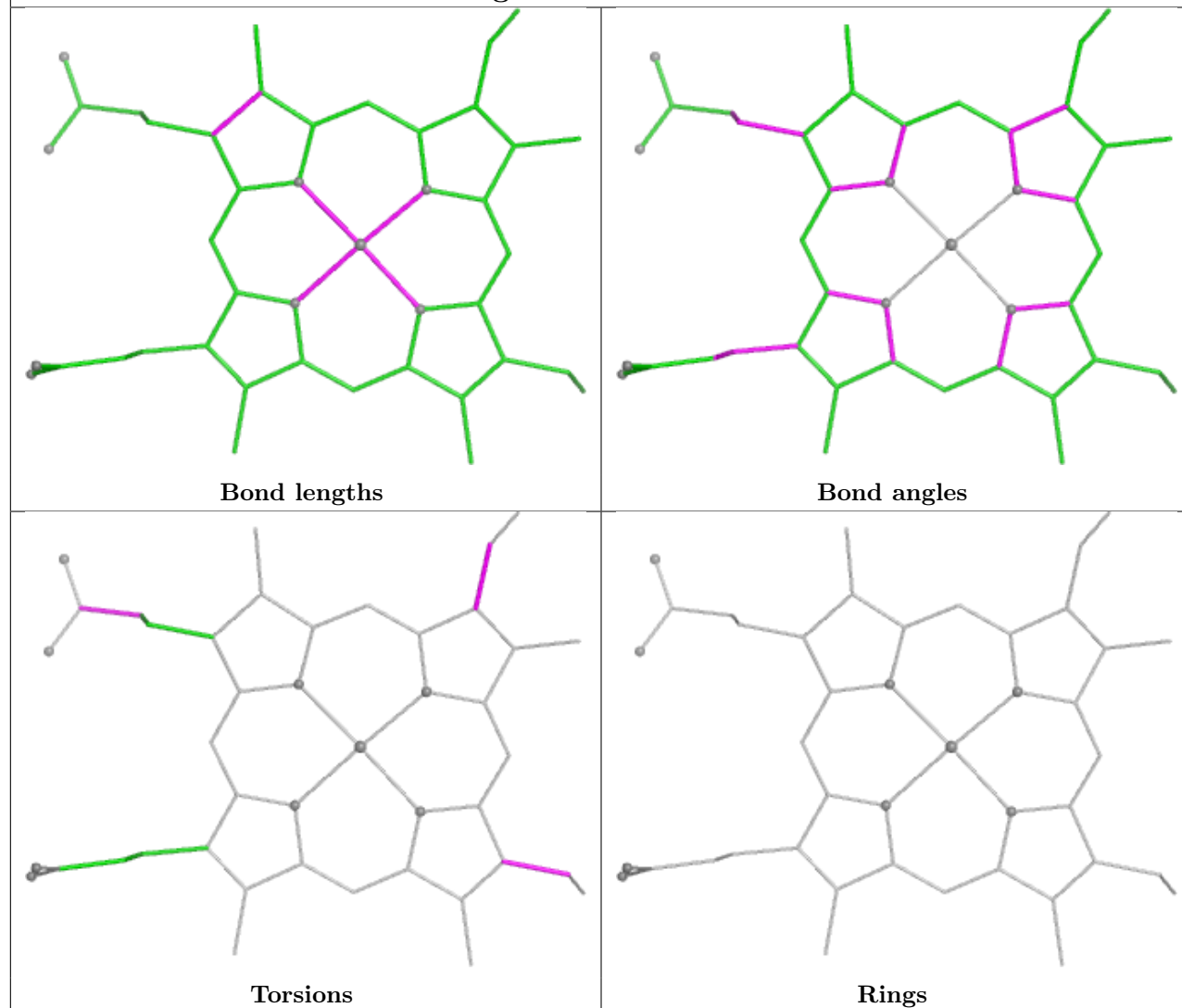
11 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1015	HAS	7	0
11	E	587	HEC	2	0
8	A	1300	7E8	1	0
8	A	1301	7E8	1	0
7	A	1200	4AG	1	0
4	A	900	5PL	5	0
5	D	1016	HAS	13	0
11	B	587	HEC	2	0
4	D	900	5PL	4	0
5	A	1016	HAS	7	0
5	A	1015	HAS	9	0

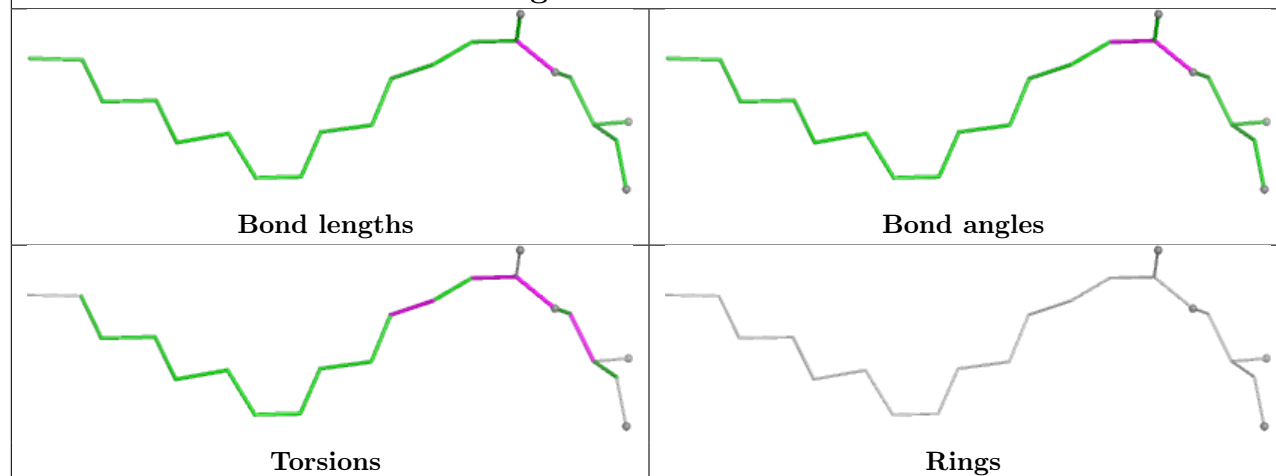
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

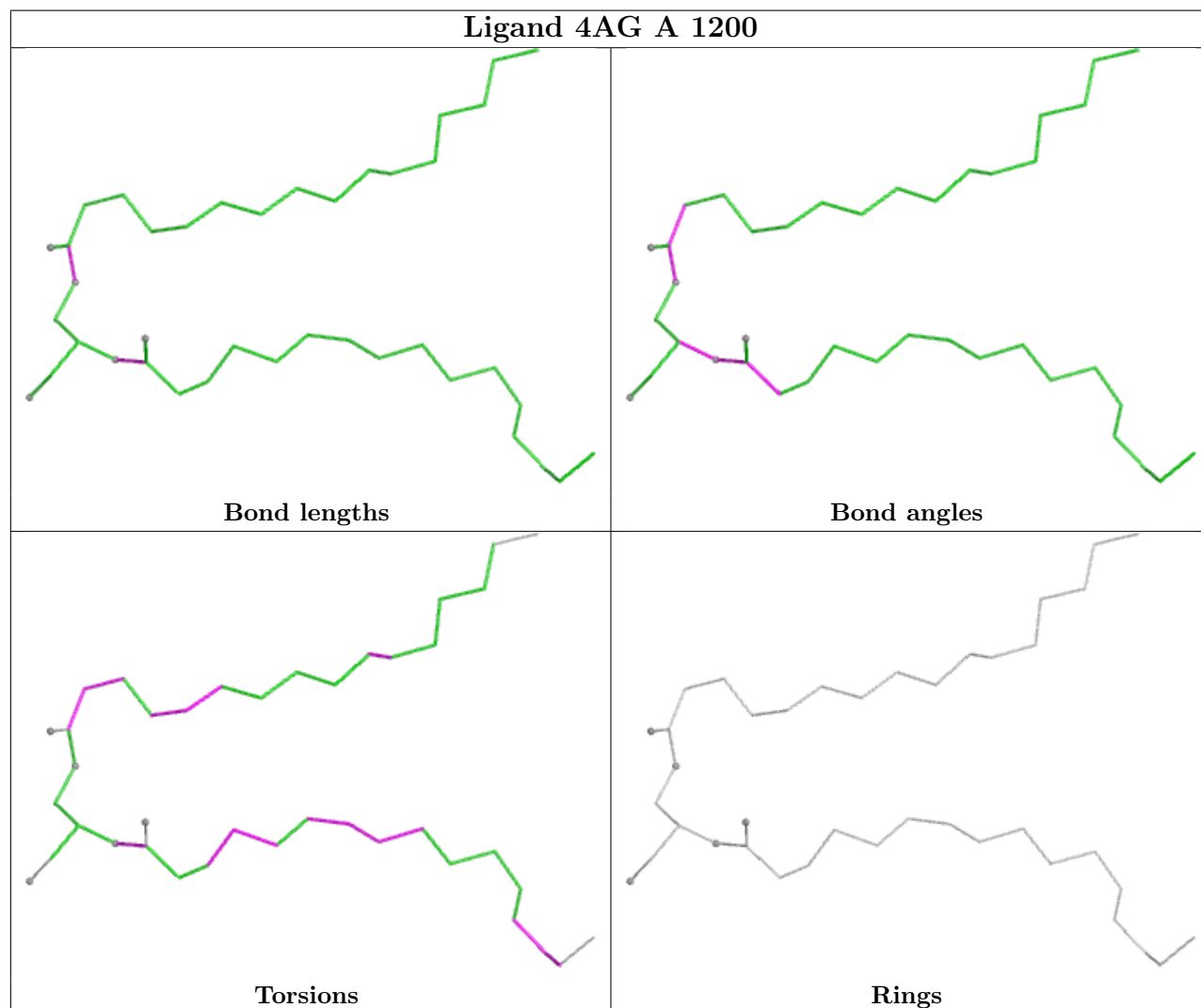
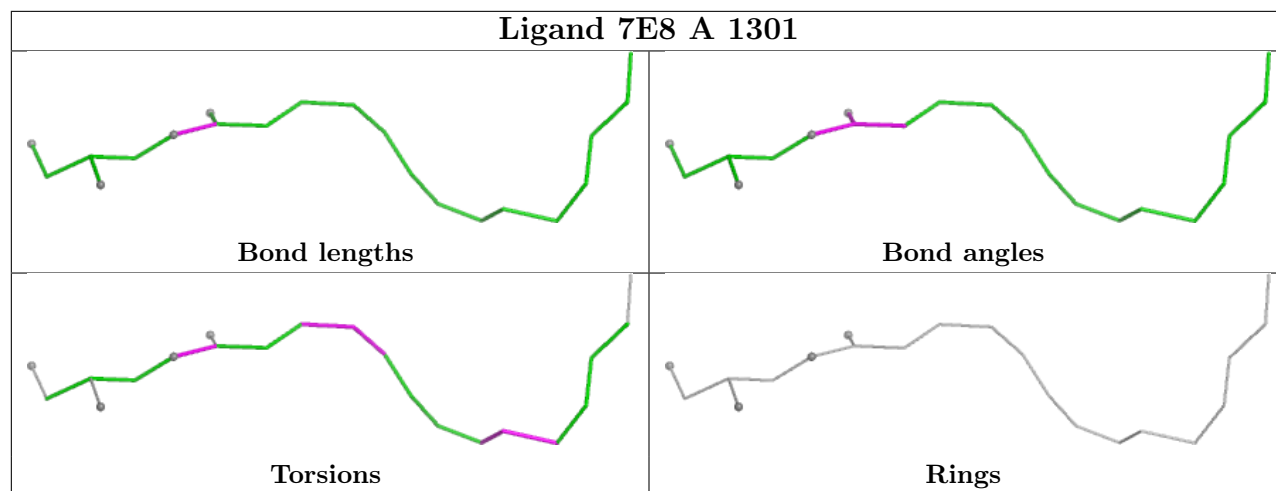


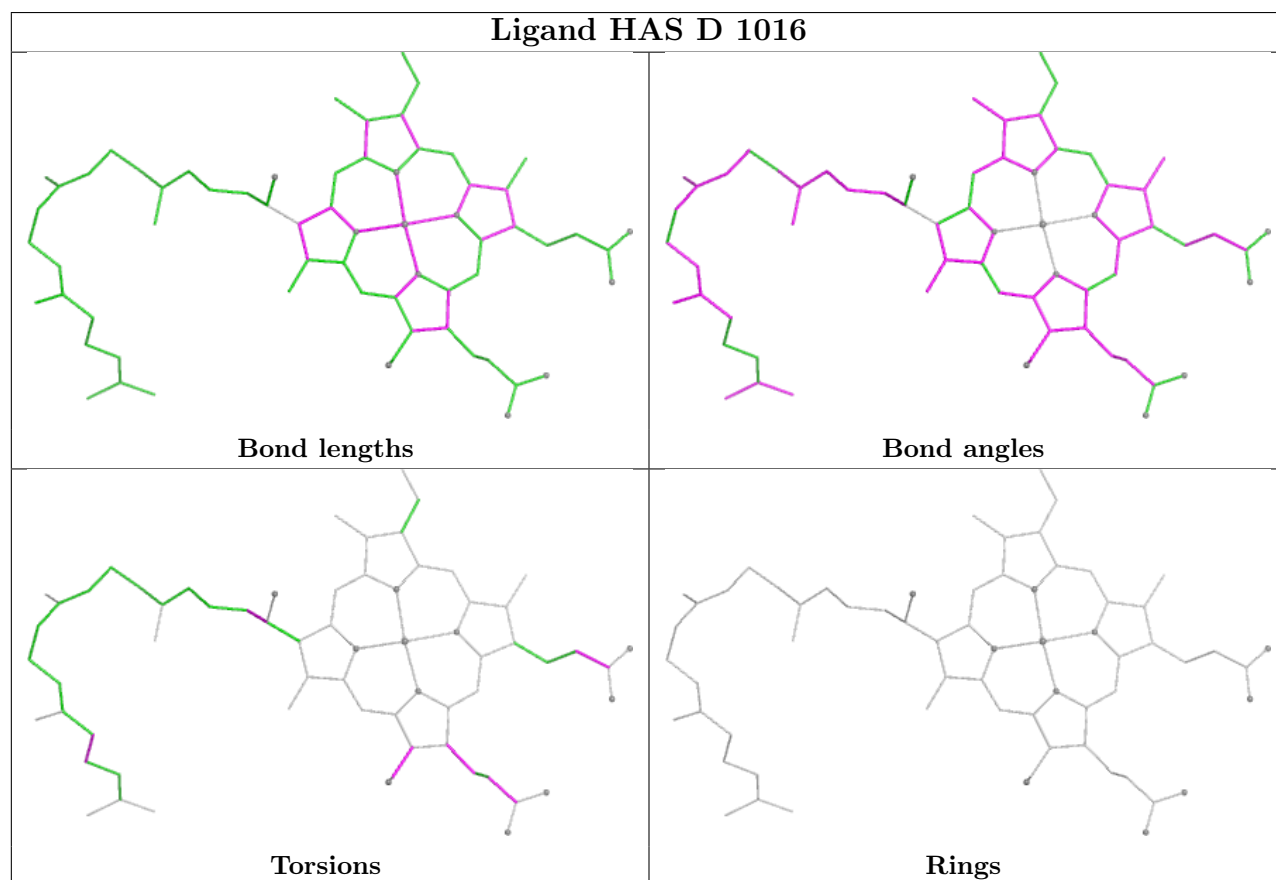
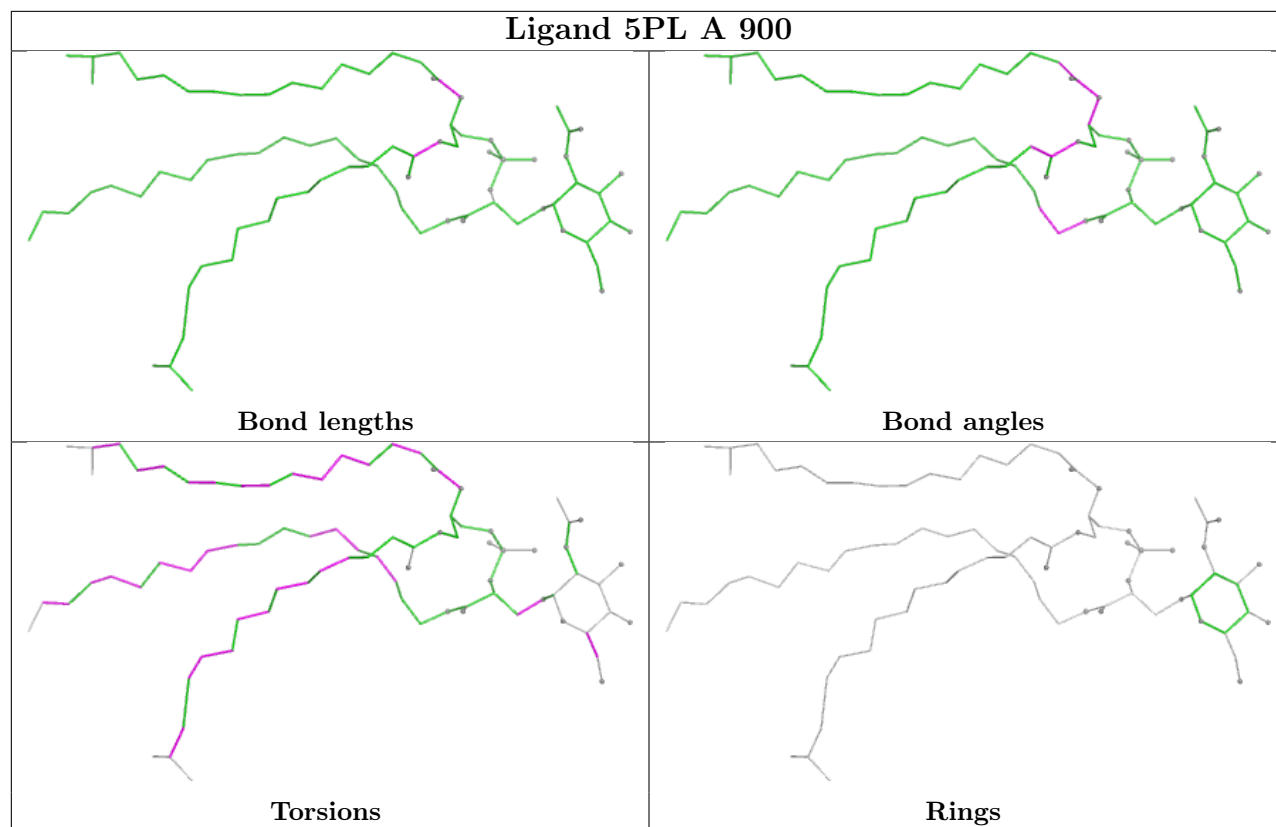
Ligand HEC E 587

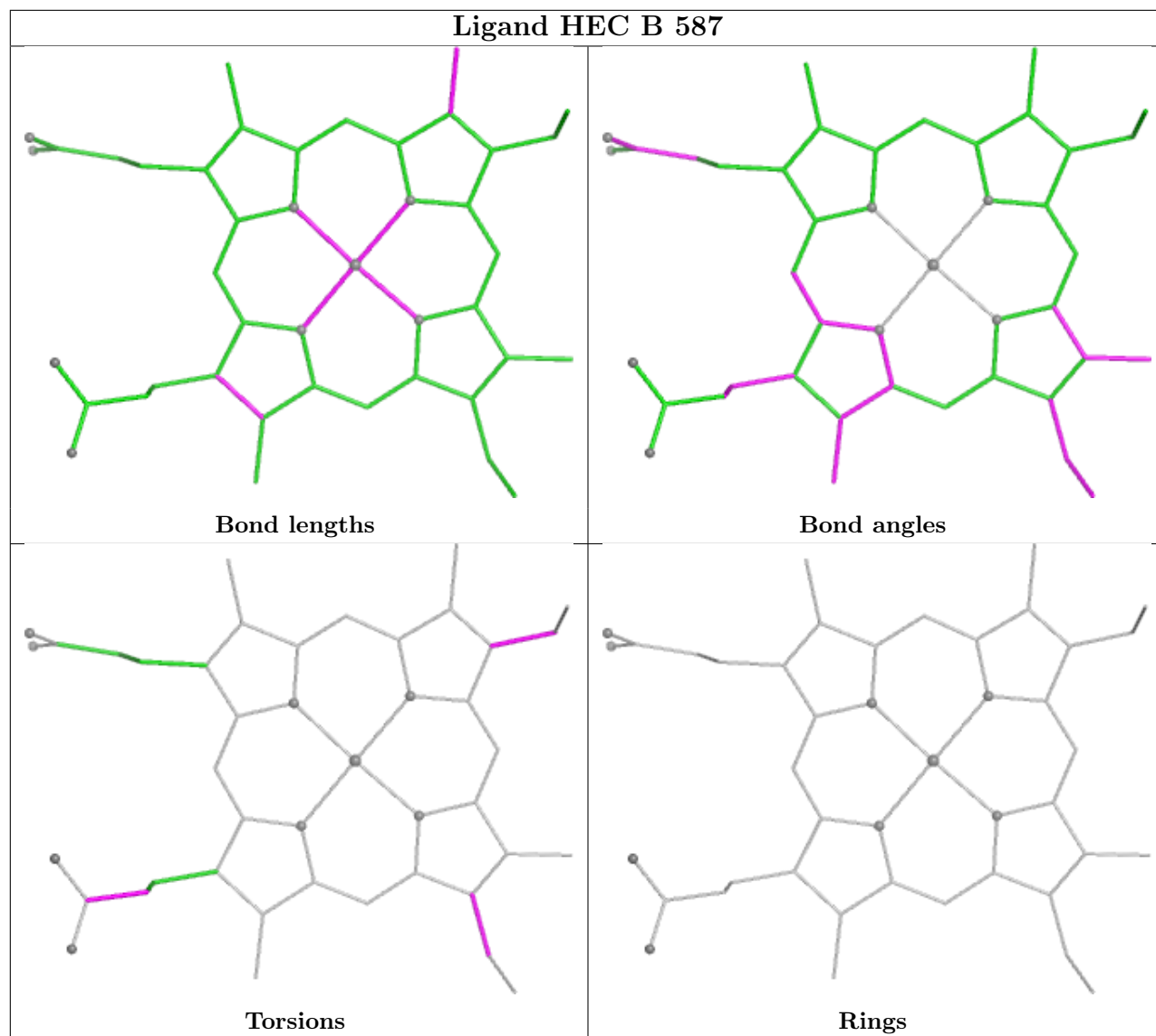


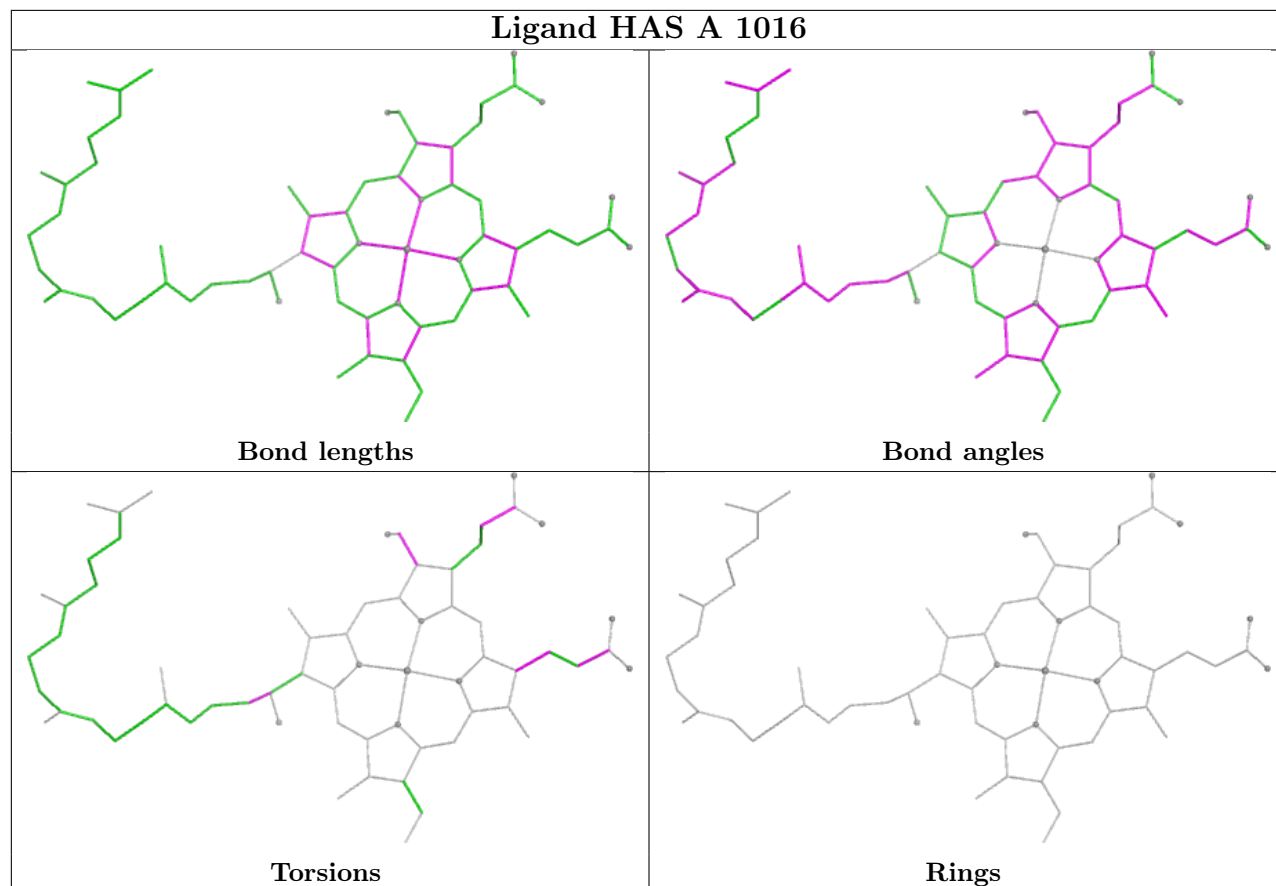
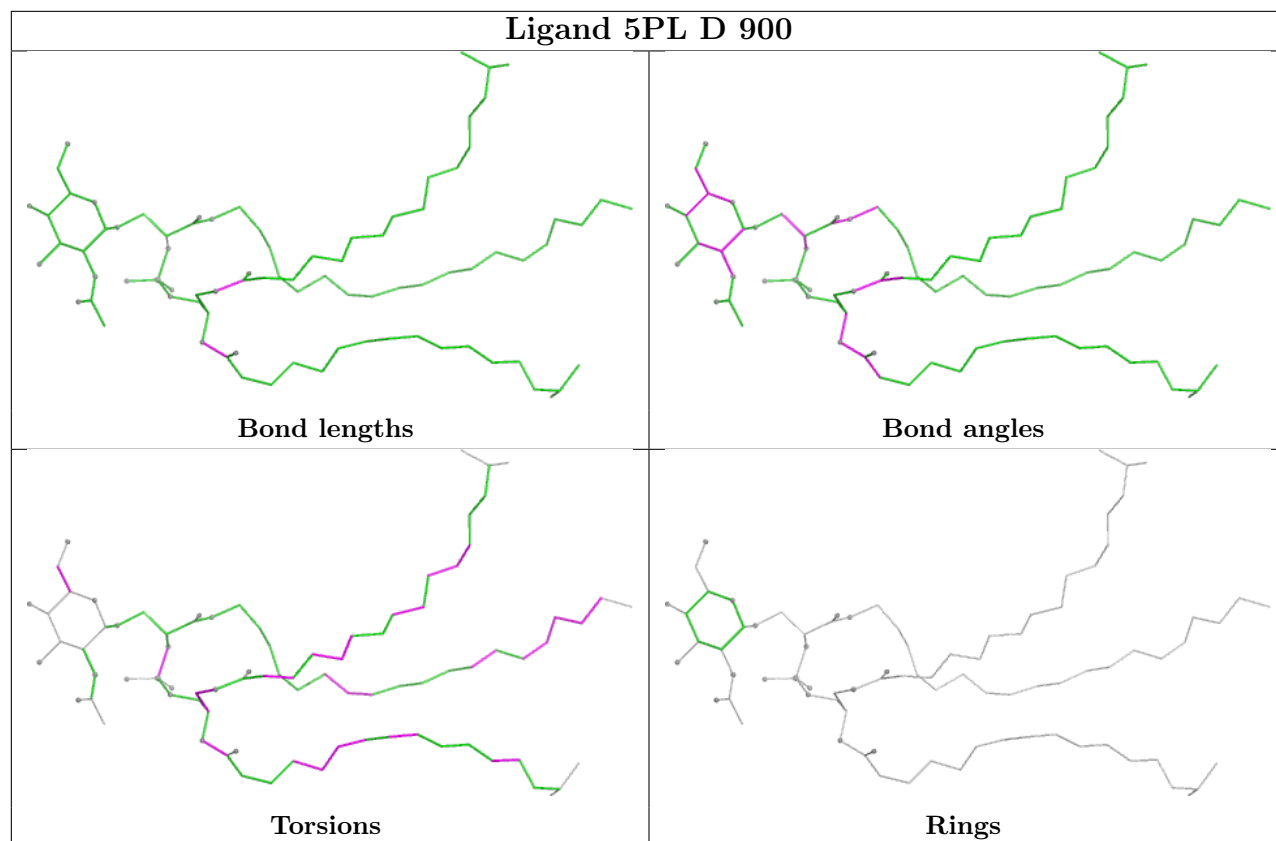
Ligand 7E8 A 1300

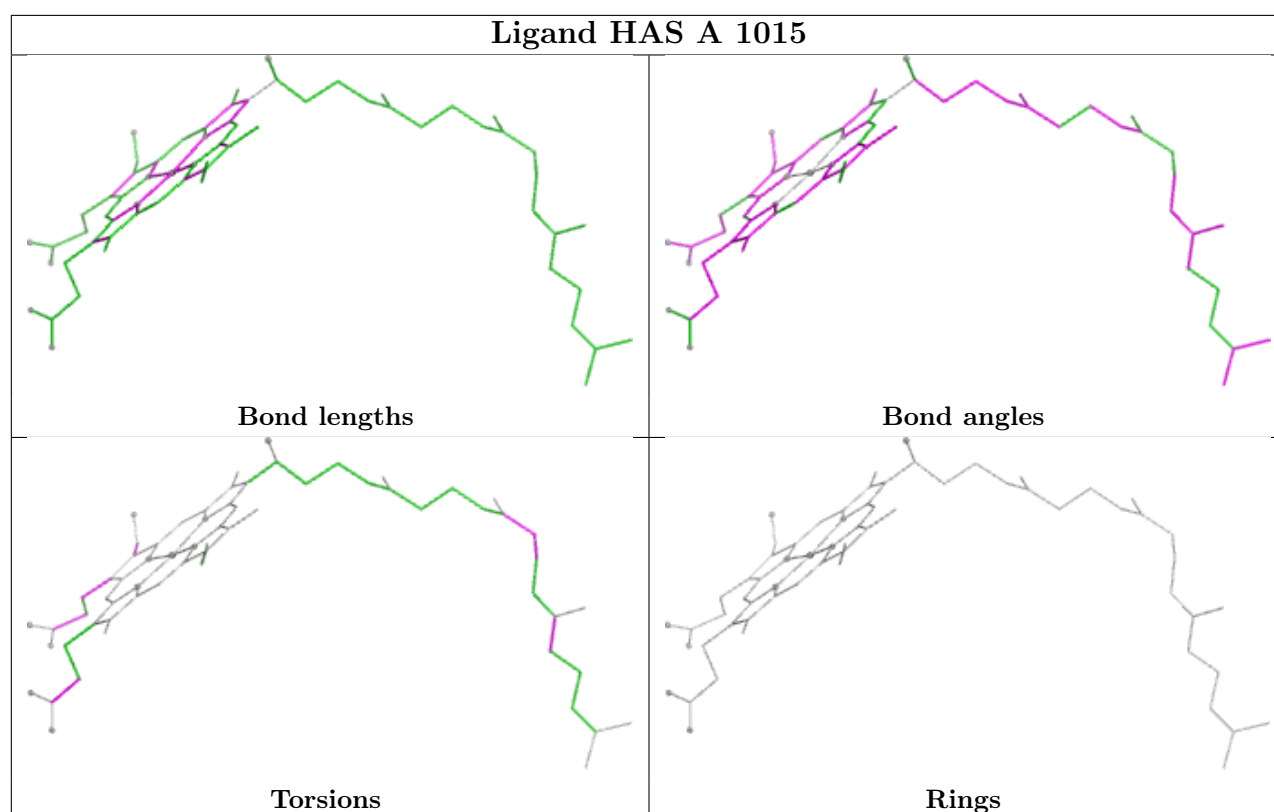
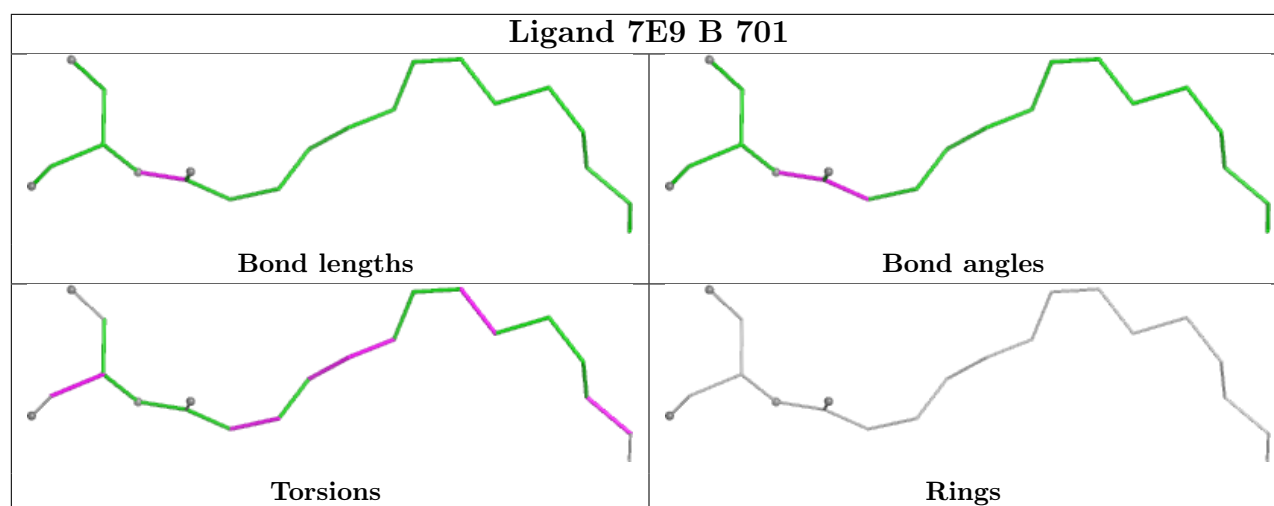












5.7 Other polymers [i](#)

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	780/791 (98%)	-0.20	7 (0%)	81 84	32, 47, 91, 174	1 (0%)
1	D	780/791 (98%)	-0.20	7 (0%)	81 84	33, 53, 89, 153	0
2	B	319/337 (94%)	-0.17	1 (0%)	90 92	33, 50, 85, 163	0
2	E	319/337 (94%)	0.09	5 (1%)	70 76	38, 67, 105, 189	0
3	C	63/66 (95%)	0.39	4 (6%)	26 29	44, 62, 112, 152	0
3	F	62/66 (93%)	0.30	1 (1%)	70 76	45, 65, 104, 153	0
All	All	2323/2388 (97%)	-0.13	25 (1%)	78 82	32, 53, 94, 189	1 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	12	TRP	4.6
1	A	691	PHE	3.7
2	E	23	ALA	3.4
1	A	539	VAL	3.4
1	D	103	ASP	3.0
1	A	12	TRP	2.9
1	D	591	TYR	2.8
2	E	25	THR	2.7
3	F	31	GLY	2.6
1	A	103[A]	ASP	2.6
1	A	591	TYR	2.6
2	B	68	PRO	2.5
1	D	471	TYR	2.5
3	C	32	GLU	2.4
2	E	71	GLN	2.4
1	D	534	TRP	2.4
3	C	33	THR	2.3
3	C	22	LEU	2.2
1	A	548	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	172	ALA	2.2
1	D	452	TYR	2.2
2	E	68	PRO	2.1
2	E	72	GLU	2.1
3	C	64	HIS	2.1
1	D	183	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
3	FME	F	1	10/11	0.81	0.14	72,91,112,160	0
3	FME	C	1	10/11	0.84	0.12	69,92,107,171	0

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
12	7E9	B	701	21/21	0.86	0.18	58,90,108,109	0
8	7E8	A	1300	21/21	0.87	0.18	48,79,102,115	0
8	7E8	A	1301	21/21	0.89	0.15	44,80,96,118	0
7	4AG	A	1200	40/40	0.91	0.17	33,68,115,123	0
4	5PL	D	900	85/85	0.91	0.14	37,62,107,128	0
4	5PL	A	900	85/85	0.92	0.14	35,65,105,134	0
5	HAS	D	1015	65/65	0.95	0.12	30,55,128,138	0
13	CL	D	1701	1/1	0.95	0.15	86,86,86,86	0
11	HEC	E	587	43/43	0.96	0.10	21,54,80,91	0
13	CL	F	101	1/1	0.96	0.21	70,70,70,70	0

Continued on next page...

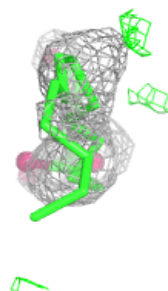
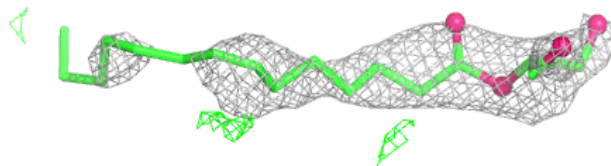
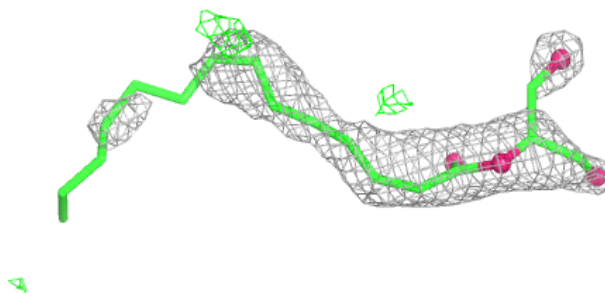
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	HAS	D	1016	65/65	0.97	0.09	24,47,86,103	0
5	HAS	A	1015	65/65	0.97	0.11	24,35,102,151	0
9	MG	D	1801	1/1	0.98	0.10	50,50,50,50	0
11	HEC	B	587	43/43	0.98	0.06	22,34,48,52	0
5	HAS	A	1016	65/65	0.98	0.07	22,38,59,62	0
13	CL	C	101	1/1	0.99	0.15	60,60,60,60	0
10	CUA	E	585	2/2	0.99	0.03	43,43,43,44	0
9	MG	A	1801	1/1	0.99	0.09	39,39,39,39	0
6	CU	A	1017	1/1	1.00	0.03	37,37,37,37	0
10	CUA	B	585	2/2	1.00	0.03	35,35,35,36	0
6	CU	D	1017	1/1	1.00	0.02	42,42,42,42	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.

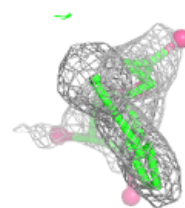
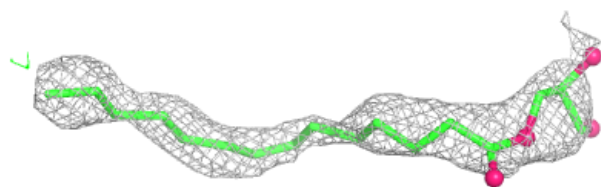
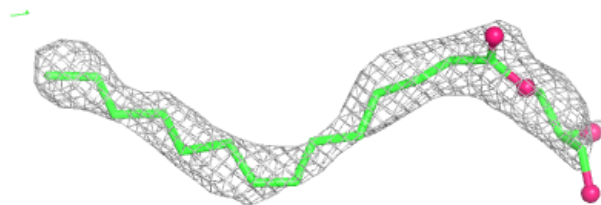
Electron density around 7E9 B 701:

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

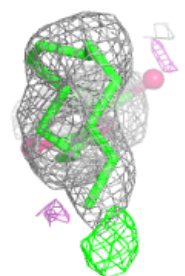
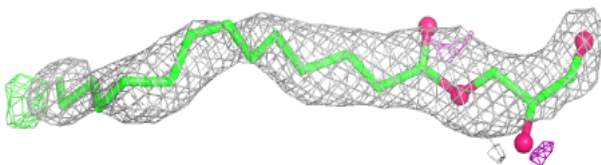
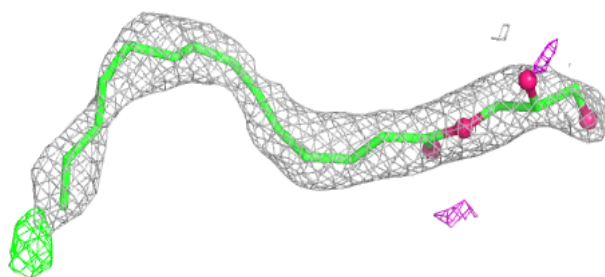


Electron density around 7E8 A 1300:

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

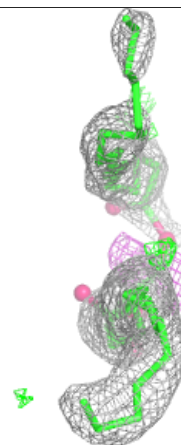
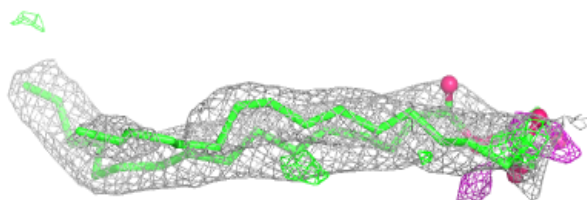
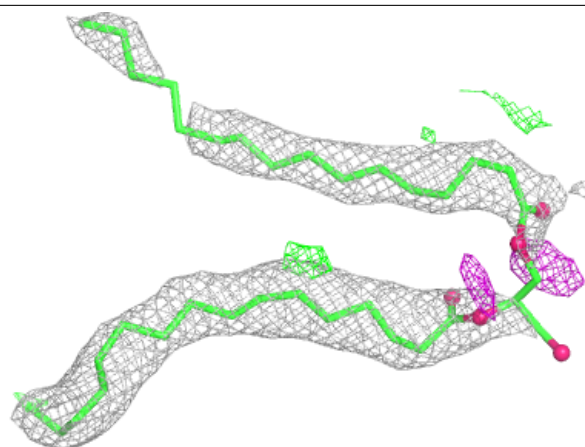
**Electron density around 7E8 A 1301:**

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

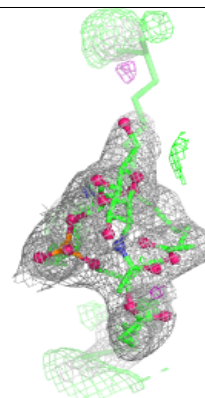
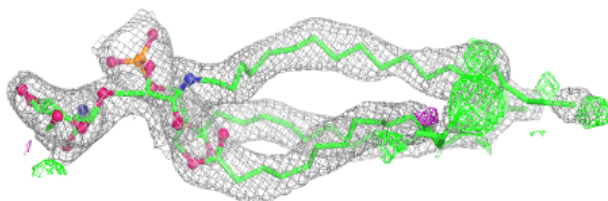
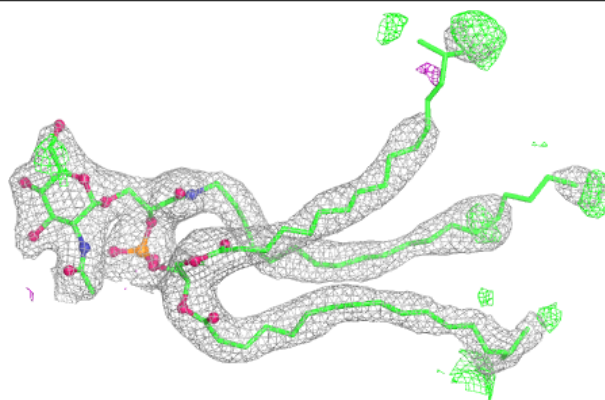


Electron density around 4AG A 1200:

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

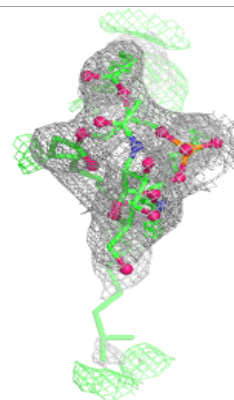
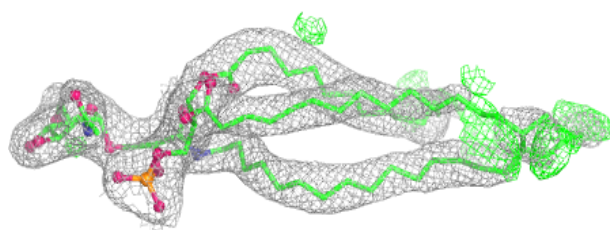
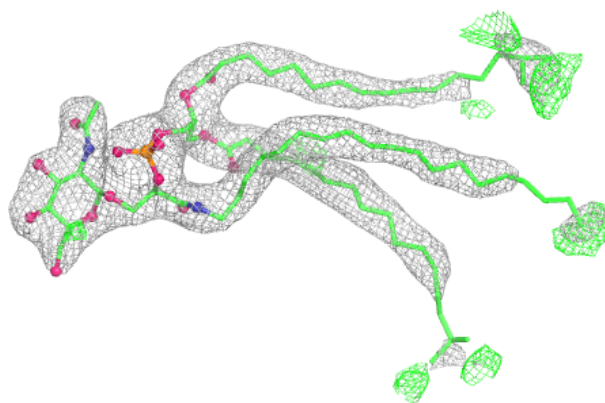
**Electron density around 5PL D 900:**

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

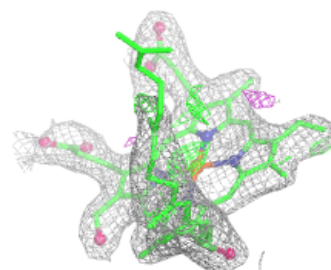
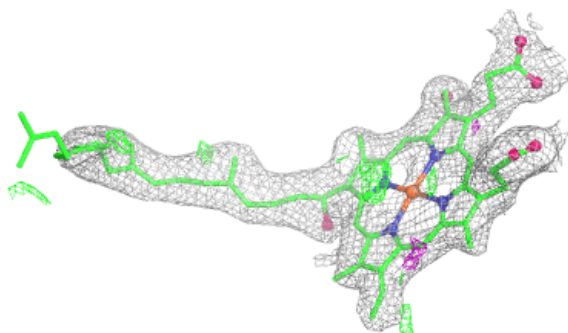
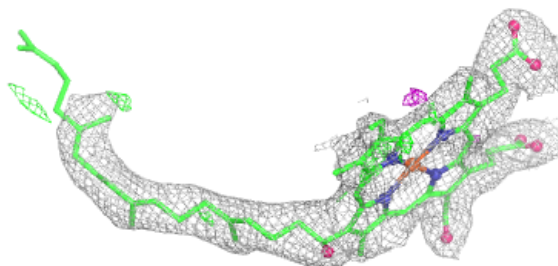


Electron density around 5PL A 900:

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

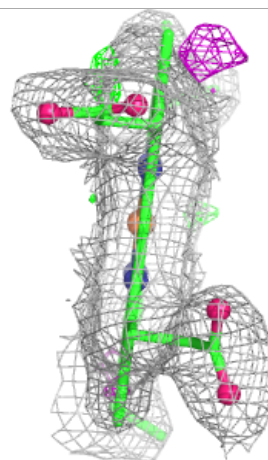
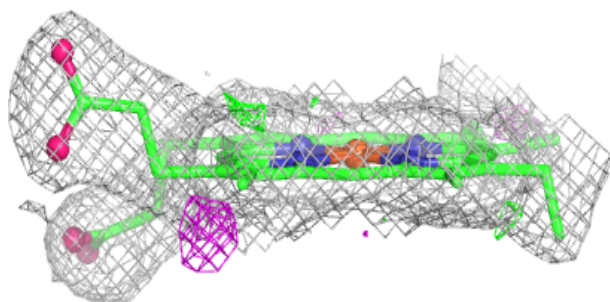
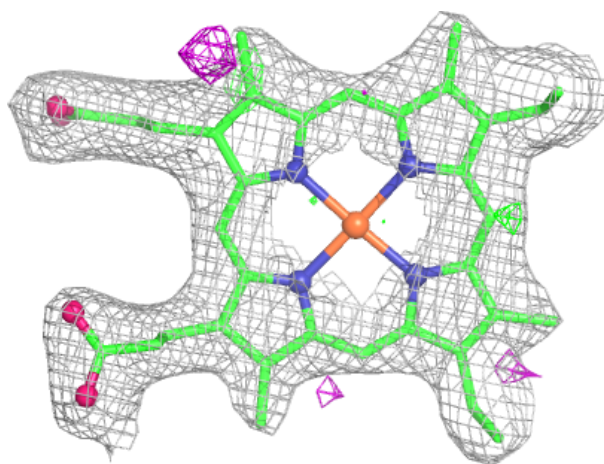
**Electron density around HAS D 1015:**

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



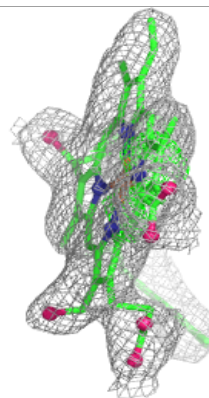
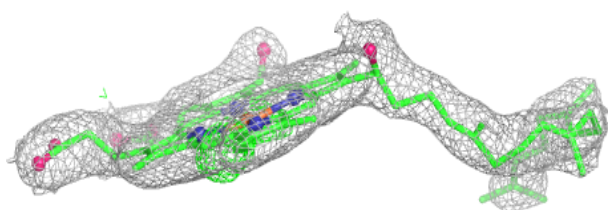
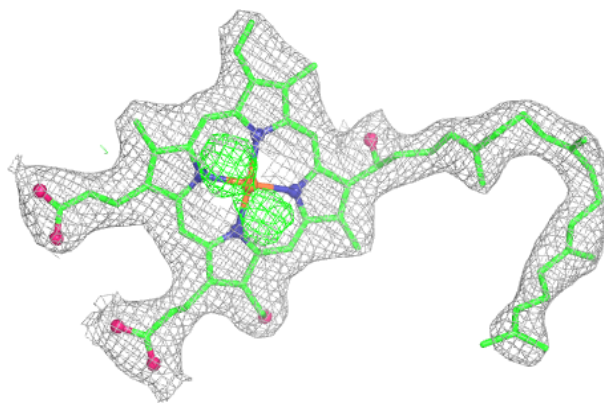
Electron density around HEC E 587:

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

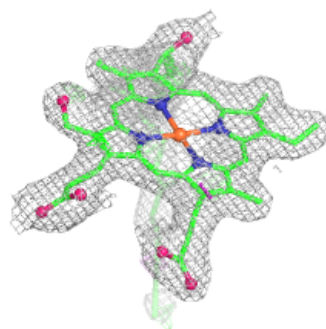
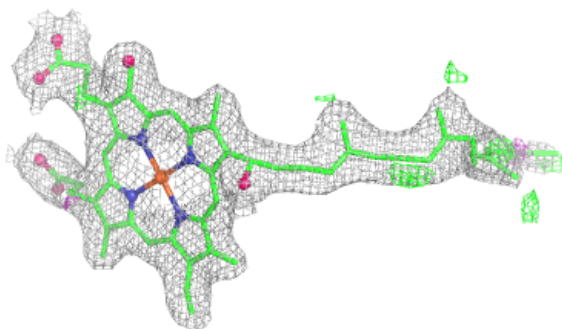
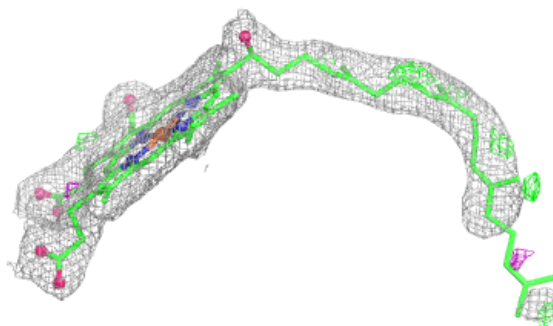


Electron density around HAS D 1016:

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

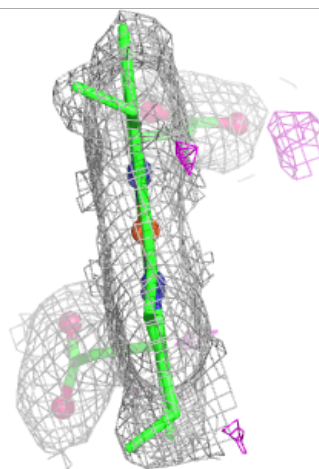
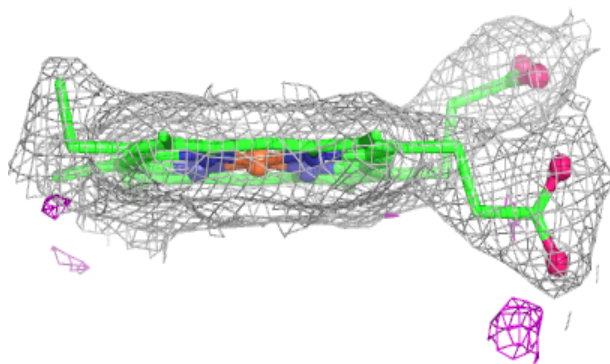
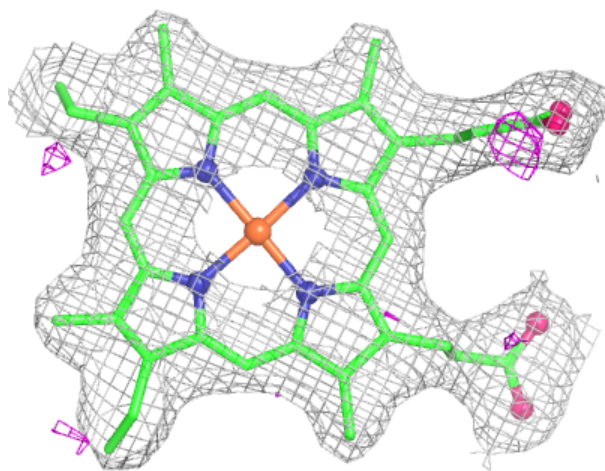
**Electron density around HAS A 1015:**

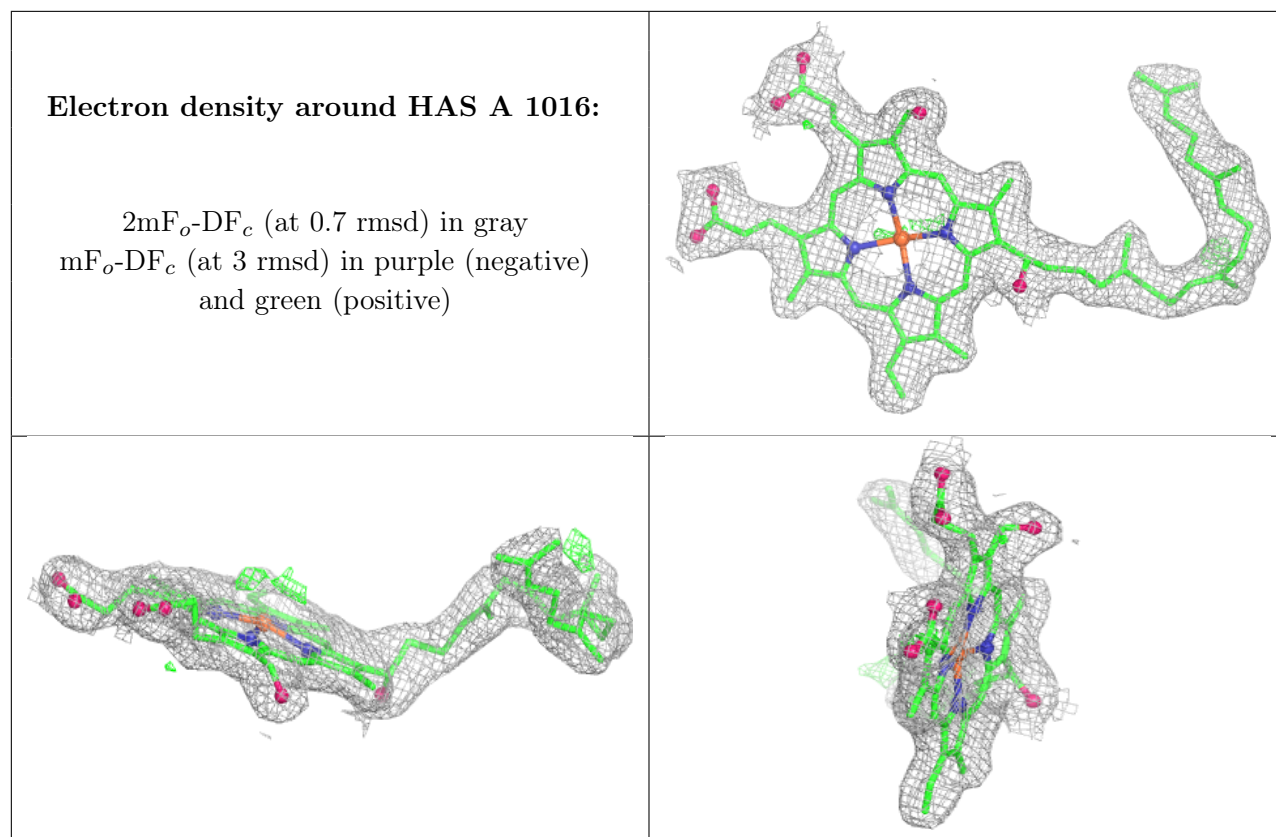
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC B 587:

$2mF_o-DF_c$ (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.