



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 07:21 AM EDT

PDB ID : 6NSW
Title : X-ray reduced Catalase 3 From N.Crassa in Cpd I state (0.135 MGy)
Authors : Zarate-Romero, A.; Rudino-Pinera, E.; Stojanoff, V.
Deposited on : 2019-01-25
Resolution : 2.10 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

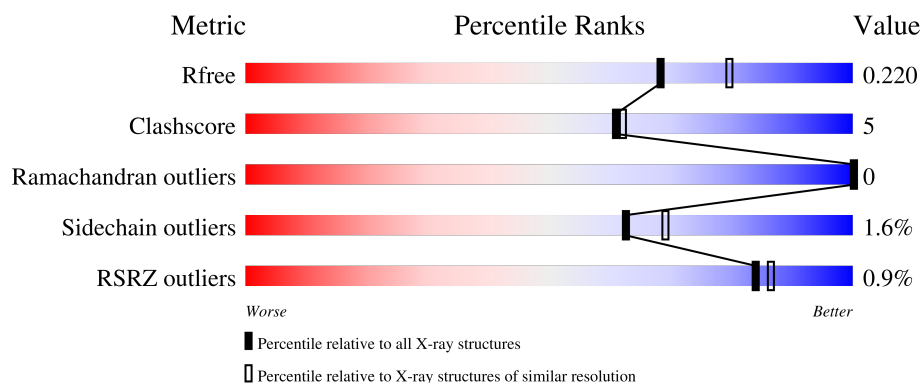
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	719	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 10%, green 85%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 85% 10% 5% </div> </div>
1	B	719	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 83%, yellow 11%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 83% 11% 6% </div> </div>
1	C	719	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 9%, green 85%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 85% 9% 6% </div> </div>
1	D	719	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 9%, green 85%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 85% 9% 6% </div> </div>

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
8	EOH	D	809	-	-	X	-

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



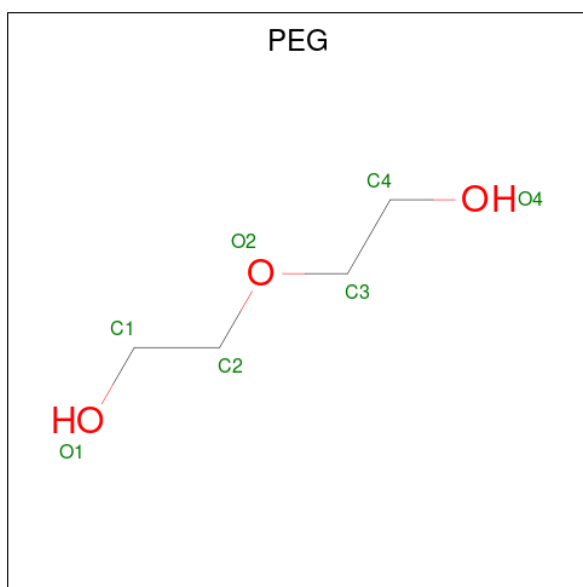
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



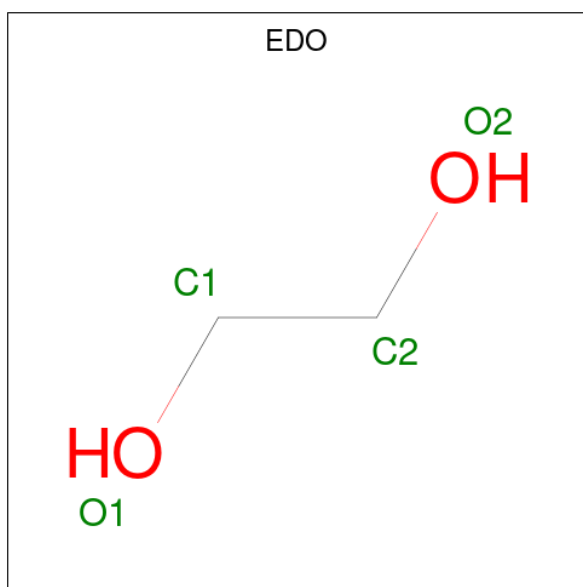
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

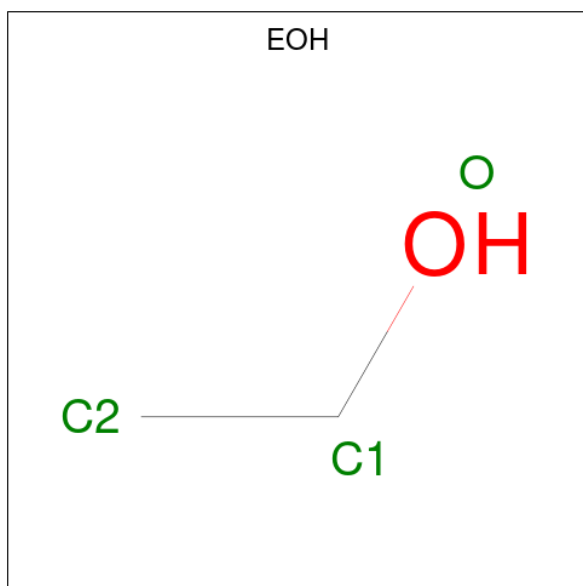
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is OXYGEN ATOM (three-letter code: O) (formula: O) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		
7	B	1	Total	O	0	0
			1	1		
7	C	1	Total	O	0	0
			1	1		
7	D	1	Total	O	0	0
			1	1		

- Molecule 8 is ETHANOL (three-letter code: EOH) (formula: C₂H₆O).



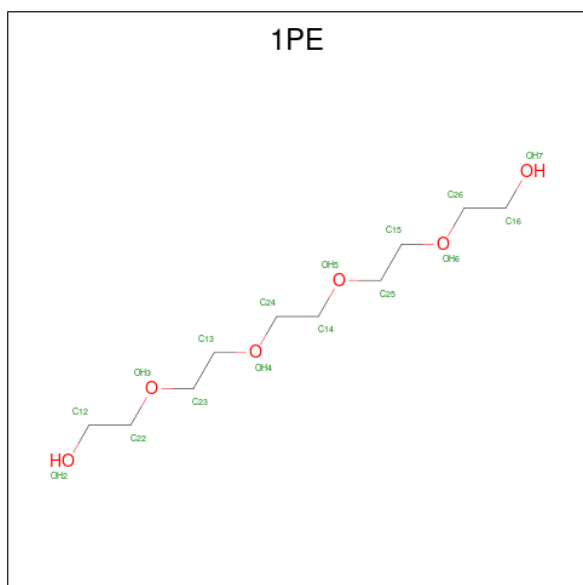
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			3	2	1		
8	B	1	Total	C	O	0	0
			3	2	1		
8	B	1	Total	C	O	0	0
			3	2	1		

Continued on next page...

Continued from previous page...

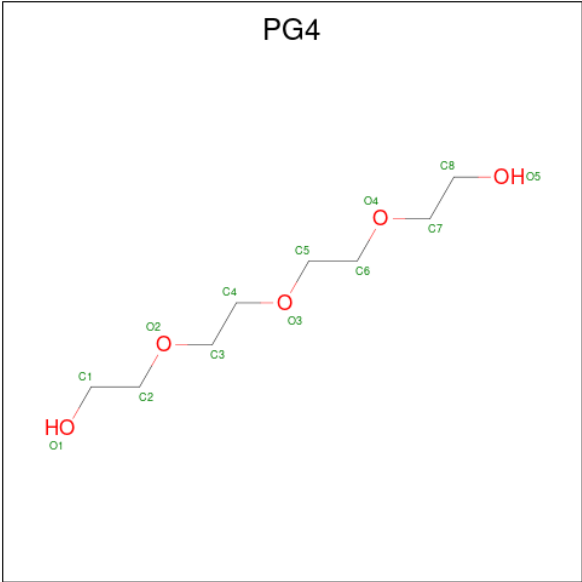
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			3	2	1		
8	D	1	Total	C	O	0	0
			3	2	1		

- Molecule 9 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 10 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			13	8	5		

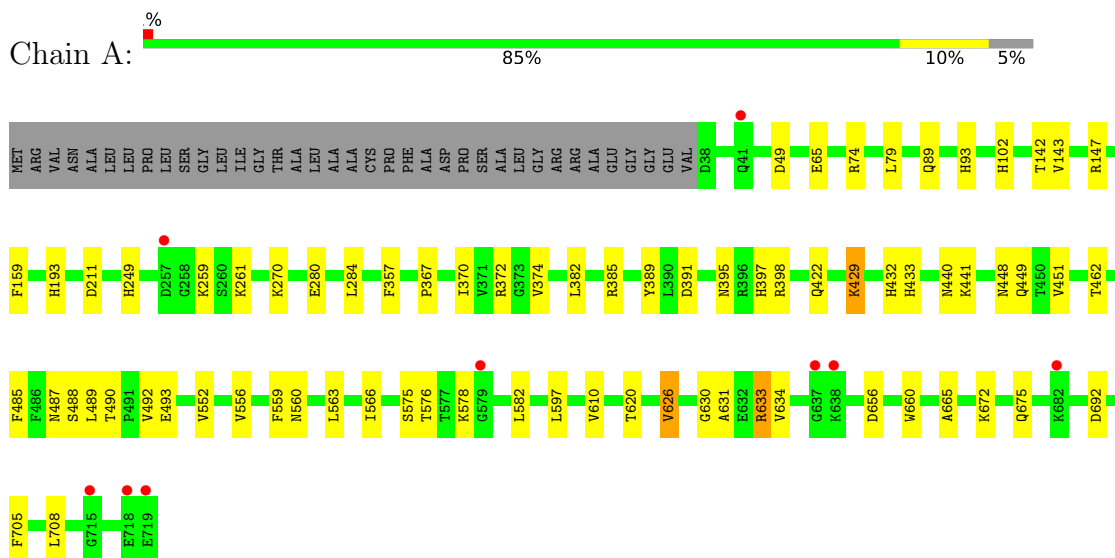
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	493	Total	O	0	0
			493	493		
11	B	502	Total	O	0	0
			502	502		
11	C	499	Total	O	0	0
			499	499		
11	D	473	Total	O	0	0
			473	473		

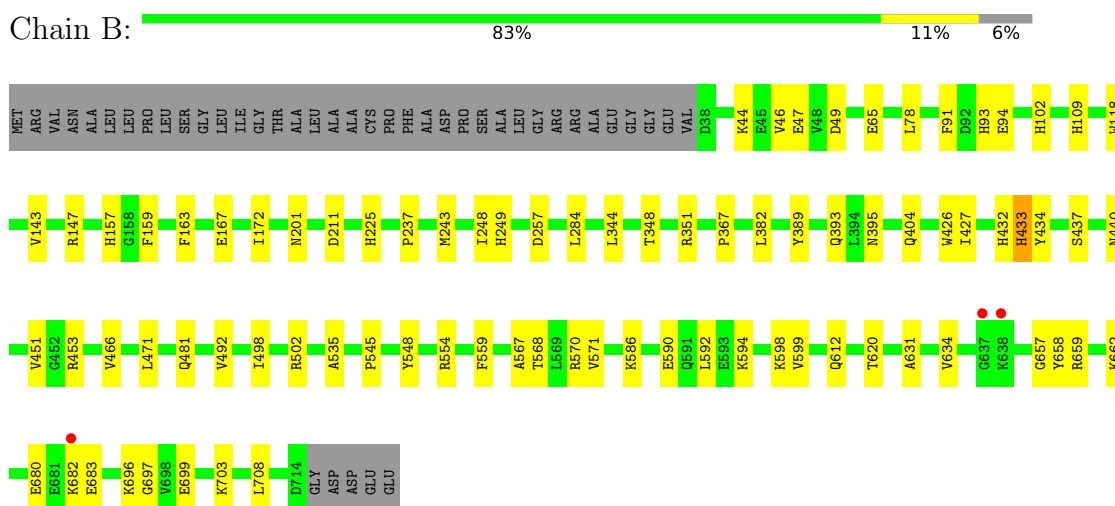
3 Residue-property plots [i](#)

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.

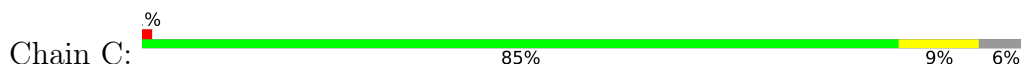
• Molecule 1: Catalase-3

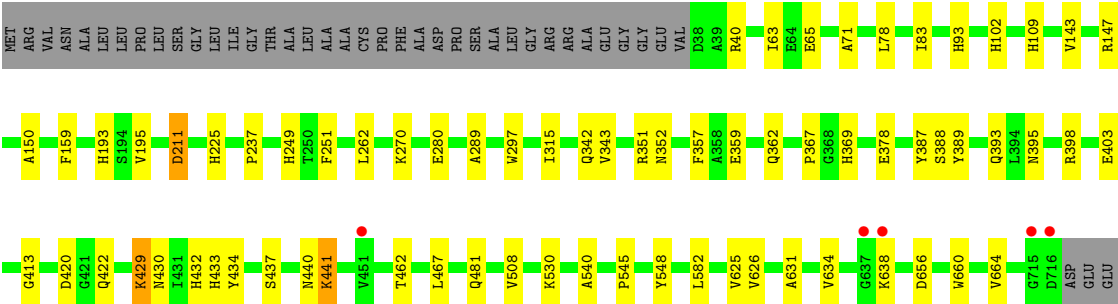


• Molecule 1: Catalase-3

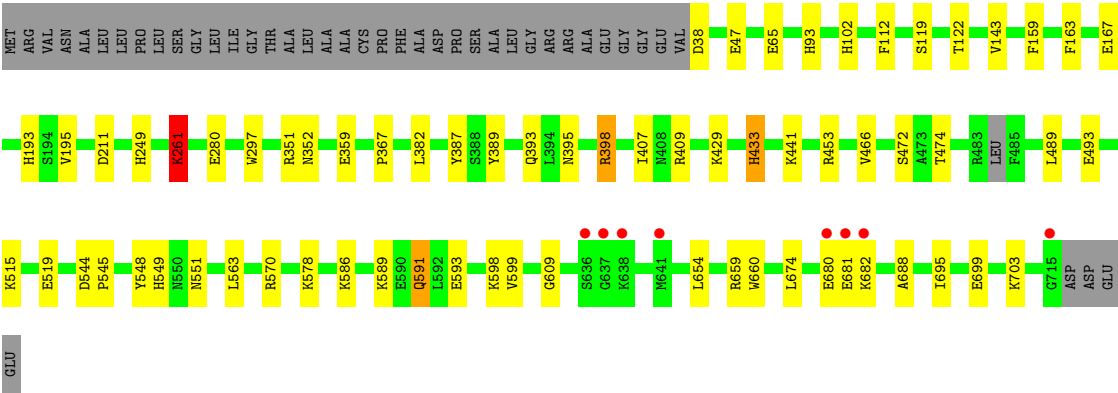
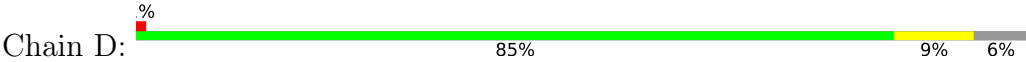


• Molecule 1: Catalase-3





● Molecule 1: Catalase-3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	131.10Å 154.40Å 160.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.60 – 2.10 29.60 – 2.10	Depositor EDS
% Data completeness (in resolution range)	80.5 (29.60-2.10) 80.6 (29.60-2.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.12 _2829	Depositor
R, R_{free}	0.170 , 0.220 0.170 , 0.220	Depositor DCC
R_{free} test set	7671 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.023 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23881	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: 1PE, ACT, HEM, EDO, PG4, O, PEG, PGE, EOH

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	0.27	0/5544	0.46	0/7520
1	B	0.27	0/5502	0.46	0/7462
1	C	0.27	0/5544	0.45	0/7517
1	D	0.28	1/5512 (0.0%)	0.45	0/7471
All	All	0.27	1/22102 (0.0%)	0.46	0/29970

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	261	LYS	CE-NZ	7.15	1.67	1.49

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	5410	0	5218	58	0
1	B	5366	0	5195	52	0
1	C	5411	0	5227	53	0
1	D	5377	0	5201	52	0
2	A	43	0	30	1	0
2	B	43	0	30	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	43	0	30	1	0
2	D	43	0	30	1	0
3	A	8	0	6	0	0
3	B	8	0	6	0	0
3	C	8	0	6	2	0
3	D	8	0	6	1	0
4	A	10	0	14	0	0
4	B	10	0	14	1	0
4	D	10	0	14	1	0
5	A	7	0	10	0	0
5	C	21	0	30	0	0
6	A	8	0	12	1	0
6	B	8	0	12	0	0
6	C	12	0	18	1	0
6	D	12	0	18	1	0
7	A	1	0	0	0	0
7	B	1	0	0	1	0
7	C	1	0	0	1	0
7	D	1	0	0	0	0
8	A	3	0	6	0	0
8	B	6	0	12	0	0
8	D	6	0	12	2	0
9	B	16	0	22	1	0
10	C	13	0	18	4	0
11	A	493	0	0	4	0
11	B	502	0	0	3	0
11	C	499	0	0	8	0
11	D	473	0	0	2	0
All	All	23881	0	21197	194	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 5.

All (194) 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)
7:C:811:O:O	11:C:901:HOH:O	1.90	0.88
1:D:659:ARG:HH12	4:D:804:PGE:H3	1.47	0.79
1:D:591:GLN:OE1	1:D:695:ILE:HG21	1.89	0.71
1:A:488:SER:HB2	1:A:556:VAL:HG11	1.75	0.69
1:B:594:LYS:HE2	1:B:594:LYS:HA	1.74	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147[A]:ARG:NH2	11:C:906:HOH:O	2.26	0.67
1:C:433:HIS:CE1	1:D:193:HIS:HB3	2.30	0.67
1:A:397:HIS:HA	1:C:422:GLN:HE22	1.60	0.66
1:B:657:GLY:HA2	1:B:662:LYS:HD2	1.76	0.66
1:D:280:GLU:HB2	1:D:660:TRP:CD2	2.32	0.65
1:B:682:LYS:HD2	1:B:682:LYS:N	2.12	0.65
1:B:237:PRO:HG3	1:B:243:MET:HE3	1.78	0.65
1:B:659:ARG:HH12	9:B:804:1PE:H132	1.62	0.64
1:D:195[A]:VAL:HG21	3:D:802:ACT:H1	1.80	0.64
1:B:147[A]:ARG:O	11:B:901:HOH:O	2.15	0.64
2:A:801:HEM:HMB2	2:A:801:HEM:HBB2	1.81	0.63
1:C:342:GLN:HG2	10:C:804:PG4:H32	1.80	0.63
1:A:49:ASP:HA	1:C:429:LYS:HG2	1.80	0.62
1:D:409:ARG:HH22	8:D:809:EOH:H12	1.63	0.62
1:A:193:HIS:HB3	1:B:433:HIS:CE1	2.35	0.61
1:A:398:ARG:HE	1:D:398:ARG:HE	1.48	0.61
1:D:38:ASP:HA	1:D:351:ARG:HH21	1.65	0.60
1:C:71:ALA:HB2	1:C:78:LEU:HD21	1.84	0.60
1:C:193:HIS:HB3	1:D:433:HIS:CE1	2.37	0.60
1:C:398:ARG:NH2	11:C:911:HOH:O	2.35	0.59
2:D:801:HEM:HMB2	2:D:801:HEM:HBB2	1.84	0.59
1:C:530:LYS:HG2	1:C:540:ALA:HB1	1.84	0.59
7:B:808:O:O	11:B:902:HOH:O	2.17	0.58
1:C:63:ILE:HD12	1:C:83:ILE:HG23	1.85	0.58
1:B:163:PHE:HE1	1:B:172:ILE:HD12	1.68	0.58
1:B:586:LYS:NZ	1:B:590:GLU:OE2	2.37	0.57
1:A:398:ARG:HE	1:D:398:ARG:NE	2.02	0.56
1:A:261:LYS:NZ	11:A:902:HOH:O	2.31	0.56
1:B:167:GLU:OE2	1:B:453:ARG:NE	2.31	0.56
1:A:93:HIS:CD2	1:D:395:ASN:HB2	2.41	0.56
1:B:571:VAL:HB	1:B:599:VAL:HG22	1.88	0.56
1:C:429:LYS:HE3	1:C:430:ASN:HB2	1.88	0.55
1:D:167:GLU:OE2	1:D:453:ARG:NE	2.40	0.54
1:A:485:PHE:CE1	1:A:556:VAL:HG22	2.43	0.54
1:D:586:LYS:NZ	1:D:609:GLY:O	2.23	0.54
1:D:544:ASP:OD2	11:D:901:HOH:O	2.19	0.54
1:A:357:PHE:CE1	1:C:420:ASP:HA	2.44	0.53
1:D:695:ILE:O	1:D:699:GLU:HG3	2.07	0.53
1:A:626[B]:VAL:HG22	1:A:665:ALA:HB3	1.90	0.53
1:A:630:GLY:O	1:A:633:ARG:HG2	2.06	0.53
1:A:280:GLU:HB2	1:A:660:TRP:CD2	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:GLU:HB3	1:D:429:LYS:HE3	1.91	0.53
1:D:570:ARG:HG2	1:D:598:LYS:HB3	1.90	0.53
1:B:682:LYS:HD2	1:B:682:LYS:H	1.73	0.52
1:B:284:LEU:HD13	1:B:620:THR:HB	1.90	0.52
1:D:549:HIS:CE1	1:D:551:ASN:HB2	2.44	0.52
1:B:434:TYR:CE2	1:B:437:SER:HB2	2.45	0.52
1:D:359:GLU:HB3	1:D:407:ILE:HD13	1.91	0.52
1:C:395:ASN:O	1:C:398:ARG:HD3	2.10	0.52
1:C:195[A]:VAL:HG21	3:C:802:ACT:H1	1.92	0.51
1:D:389:TYR:O	1:D:393:GLN:HG2	2.10	0.51
1:C:656:ASP:HB3	1:C:660:TRP:CZ3	2.46	0.51
1:C:249:HIS:HB2	1:C:251:PHE:CE1	2.46	0.51
1:C:434:TYR:CE2	1:C:437:SER:HB2	2.45	0.50
1:C:462:THR:HG22	1:D:466:VAL:HG12	1.92	0.50
1:A:559:PHE:HB3	1:A:708:LEU:HD11	1.93	0.50
1:C:625:VAL:O	1:C:664:VAL:HA	2.11	0.50
1:B:257:ASP:OD1	1:B:257:ASP:N	2.42	0.50
1:A:462:THR:HG22	1:B:466:VAL:HG12	1.94	0.50
1:A:79:LEU:HD11	1:C:387:TYR:HB2	1.92	0.49
1:B:367:PRO:HD3	1:B:389:TYR:CD2	2.47	0.49
1:A:485:PHE:HD1	1:A:556:VAL:HG21	1.78	0.49
1:B:545:PRO:HA	1:B:548:TYR:CD2	2.47	0.49
1:C:433:HIS:CD2	1:D:193:HIS:ND1	2.81	0.49
1:C:270:LYS:NZ	11:C:914:HOH:O	2.36	0.49
10:C:804:PG4:H31	11:C:1267:HOH:O	2.12	0.49
1:B:237:PRO:HG3	1:B:243:MET:CE	2.41	0.48
1:A:249:HIS:CD2	1:A:382:LEU:HB2	2.48	0.48
1:A:563:LEU:CD2	1:A:705:PHE:HB2	2.43	0.48
1:B:93:HIS:ND1	1:C:395:ASN:HB2	2.28	0.48
1:A:672:LYS:HA	1:A:675:GLN:HG3	1.95	0.48
1:C:631:ALA:O	1:C:634:VAL:HG22	2.14	0.48
1:B:78:LEU:HD11	1:C:467:LEU:HD22	1.95	0.47
1:D:549:HIS:ND1	1:D:551:ASN:HB2	2.30	0.47
1:B:102:HIS:CE1	1:B:143:VAL:HG22	2.48	0.47
1:C:389:TYR:O	1:C:393:GLN:HG2	2.14	0.47
1:A:575:SER:HA	1:A:631:ALA:HB2	1.97	0.47
1:A:284:LEU:HD13	1:A:620:THR:HB	1.96	0.47
1:A:398:ARG:NH1	11:A:927:HOH:O	2.48	0.47
1:C:367:PRO:HD3	1:C:389:TYR:CD2	2.50	0.47
1:C:545:PRO:HA	1:C:548:TYR:CD2	2.51	0.46
1:A:49:ASP:HA	1:C:429:LYS:CG	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:489:LEU:HB3	1:D:493:GLU:HB3	1.95	0.46
1:A:385:ARG:O	1:A:389:TYR:HD1	1.98	0.46
1:A:391:ASP:OD1	1:D:93:HIS:HE1	1.97	0.46
1:A:485:PHE:HD1	1:A:556:VAL:CG2	2.28	0.46
1:D:367:PRO:HD3	1:D:389:TYR:CD2	2.51	0.46
1:D:515:LYS:O	1:D:519:GLU:HG2	2.16	0.46
1:A:432:HIS:HB2	1:A:440:ASN:HB3	1.97	0.46
1:B:46:VAL:HA	8:D:809:EOH:H22	1.97	0.46
1:A:370:ILE:HD11	1:A:374:VAL:HG12	1.97	0.46
1:C:369:HIS:NE2	1:C:403:GLU:OE2	2.47	0.46
1:B:91:PHE:HA	1:B:94:GLU:HG3	1.99	0.46
1:B:225:HIS:CE1	1:B:481:GLN:HB3	2.51	0.46
1:B:699:GLU:O	1:B:703:LYS:HD2	2.16	0.46
1:A:485:PHE:CD1	1:A:556:VAL:CG2	2.99	0.45
1:A:492:VAL:HG11	1:A:708:LEU:HB3	1.98	0.45
1:D:545:PRO:HA	1:D:548:TYR:CD2	2.51	0.45
1:A:563:LEU:HD21	1:A:705:PHE:HB2	1.98	0.45
1:A:367:PRO:HD2	1:A:389:TYR:CG	2.51	0.45
1:D:563:LEU:O	1:D:703:LYS:HD2	2.17	0.45
1:A:441:LYS:HG2	6:A:807:EDO:H22	1.98	0.45
1:A:489:LEU:HB3	1:A:493:GLU:HB3	1.98	0.45
1:C:433:HIS:CD2	1:D:193:HIS:CG	3.03	0.45
1:A:49:ASP:OD1	1:C:429:LYS:HE2	2.17	0.45
1:C:109:HIS:HB2	1:C:351:ARG:HB2	1.99	0.45
1:C:433:HIS:NE2	1:D:193:HIS:HB3	2.32	0.45
1:A:147[B]:ARG:HD2	11:A:928:HOH:O	2.16	0.44
1:A:485:PHE:CD1	1:A:556:VAL:HG22	2.52	0.44
1:B:389:TYR:O	1:B:393:GLN:HG2	2.17	0.44
1:A:422:GLN:NE2	1:C:398:ARG:HG2	2.32	0.44
1:D:589:LYS:HG3	1:D:599:VAL:HB	2.00	0.44
1:B:696:LYS:HG3	1:B:697:GLY:N	2.33	0.44
1:C:40:ARG:HH21	1:C:359:GLU:CD	2.21	0.44
1:C:150:ALA:HA	1:C:289:ALA:HB1	1.99	0.44
1:D:102:HIS:CE1	1:D:143:VAL:HG22	2.52	0.44
1:D:409:ARG:NH1	11:D:930:HOH:O	2.49	0.44
1:D:591:GLN:OE1	1:D:695:ILE:HD13	2.16	0.44
1:B:249:HIS:CD2	1:B:382:LEU:HB2	2.53	0.44
1:B:658:TYR:OH	1:B:683:GLU:OE1	2.31	0.44
1:A:372:ARG:HH12	1:A:449:GLN:HA	1.82	0.44
1:C:432:HIS:HB2	1:C:440:ASN:HB3	1.99	0.44
1:A:490:THR:CG2	1:A:560:ASN:HB3	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:631:ALA:O	1:B:634:VAL:HG22	2.17	0.44
1:C:262:LEU:HB2	1:C:315:ILE:HB	2.00	0.44
1:B:157:HIS:HB2	1:B:243:MET:HE1	2.00	0.44
1:B:395:ASN:HB2	1:C:93:HIS:ND1	2.33	0.44
10:C:804:PG4:H11	11:C:1267:HOH:O	2.17	0.44
1:C:343:VAL:HG12	11:C:1267:HOH:O	2.18	0.43
1:D:112:PHE:CG	1:D:163:PHE:HE1	2.35	0.43
1:B:612:GLN:OE1	4:B:805:PGE:H52	2.18	0.43
1:A:448:ASN:HB2	11:A:1283:HOH:O	2.18	0.43
1:C:441:LYS:HD2	1:C:441:LYS:HA	1.74	0.43
1:D:119:SER:HA	1:D:122:THR:O	2.18	0.43
1:A:448:ASN:OD1	1:A:451[A]:VAL:HG22	2.18	0.43
1:B:147[B]:ARG:HD2	11:C:951:HOH:O	2.18	0.43
1:C:225:HIS:CE1	1:C:481:GLN:HB3	2.53	0.43
1:B:498:ILE:HG22	1:B:502:ARG:HD2	2.00	0.43
1:C:413:GLY:HA2	6:C:808:EDO:H21	2.01	0.43
1:A:74:ARG:HG2	1:D:472:SER:HB2	2.00	0.43
1:A:89:GLN:HB2	1:D:387:TYR:OH	2.19	0.43
1:A:395:ASN:HB2	1:D:93:HIS:CD2	2.54	0.43
1:B:109:HIS:HB2	1:B:351:ARG:HB2	2.01	0.43
1:B:163:PHE:CE1	1:B:172:ILE:HD12	2.51	0.43
1:B:427:ILE:O	1:D:47:GLU:HA	2.18	0.43
1:B:49:ASP:HB2	1:D:429:LYS:HZ2	1.83	0.42
1:C:211:ASP:HA	1:C:508:VAL:HG13	2.01	0.42
1:D:297:TRP:CZ3	1:D:352:ASN:HB3	2.54	0.42
1:D:589:LYS:O	1:D:593:GLU:HG3	2.19	0.42
1:B:680:GLU:HB2	1:B:682:LYS:HG2	2.01	0.42
1:C:378:GLU:OE1	1:C:378:GLU:N	2.52	0.42
1:B:118:TRP:CZ2	1:B:344:LEU:HA	2.54	0.42
1:B:559:PHE:HB3	1:B:708:LEU:HD11	2.01	0.42
1:A:102:HIS:HA	1:A:142:THR:O	2.19	0.42
1:B:404:GLN:HG2	1:B:426:TRP:CZ2	2.54	0.42
1:C:237:PRO:HB3	3:C:803:ACT:H1	2.01	0.42
1:B:570:ARG:HA	1:B:598:LYS:O	2.20	0.41
1:C:102:HIS:CE1	1:C:143:VAL:HG22	2.55	0.41
1:A:575:SER:OG	1:A:576:THR:N	2.53	0.41
1:C:357:PHE:O	1:C:362:GLN:HG3	2.20	0.41
1:D:395:ASN:O	1:D:398:ARG:HD2	2.20	0.41
1:A:490:THR:OG1	1:A:493:GLU:HB2	2.19	0.41
10:C:804:PG4:H52	10:C:804:PG4:H71	1.66	0.41
1:B:248:ILE:HD11	11:B:1121:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:HIS:HB2	1:B:440:ASN:HB3	2.02	0.41
1:D:654:LEU:HD21	1:D:674:LEU:HD23	2.02	0.41
1:A:582:LEU:HD21	1:A:610:VAL:HG23	2.01	0.41
1:A:656:ASP:HB3	1:A:660:TRP:CZ3	2.56	0.41
1:C:297:TRP:CZ3	1:C:352:ASN:HB3	2.56	0.41
1:D:681:GLU:HG3	1:D:688:ALA:HB3	2.02	0.41
1:D:578:LYS:HA	1:D:578:LYS:HD3	1.89	0.41
1:D:261:LYS:HB2	1:D:261:LYS:HE2	1.81	0.41
1:A:429:LYS:HE3	1:A:429:LYS:HB3	1.71	0.41
1:B:567:ALA:O	1:B:568:THR:OG1	2.28	0.41
1:C:280:GLU:HB2	1:C:660:TRP:CD2	2.56	0.41
2:C:801:HEM:HMB1	2:C:801:HEM:HBB2	2.03	0.41
1:D:249:HIS:CG	1:D:382:LEU:HB2	2.56	0.41
1:B:492:VAL:HG11	1:B:708:LEU:HB3	2.03	0.41
1:B:502:ARG:HG2	1:B:535:ALA:CB	2.51	0.41
1:A:487:ASN:HB3	1:A:552:VAL:HG12	2.03	0.40
1:A:631:ALA:O	1:A:634:VAL:HG22	2.21	0.40
1:D:474:THR:HB	6:D:807:EDO:H21	2.02	0.40
1:D:680:GLU:OE1	1:D:682:LYS:NZ	2.53	0.40
1:A:566:ILE:HD12	1:A:597:LEU:HD21	2.03	0.40
1:A:578:LYS:HD3	1:A:633:ARG:CZ	2.51	0.40
1:B:201:ASN:HB3	1:C:297:TRP:CE3	2.56	0.40
1:A:102:HIS:CE1	1:A:143:VAL:HG22	2.56	0.40
1:C:582:LEU:HD12	1:C:582:LEU:HA	1.89	0.40
1:A:270:LYS:HA	1:A:270:LYS:HD2	1.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	688/719 (96%)	667 (97%)	21 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	682/719 (95%)	661 (97%)	21 (3%)	0	100	100
1	C	688/719 (96%)	667 (97%)	21 (3%)	0	100	100
1	D	682/719 (95%)	658 (96%)	24 (4%)	0	100	100
All	All	2740/2876 (95%)	2653 (97%)	87 (3%)	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	567/585 (97%)	557 (98%)	10 (2%)	59	65
1	B	562/585 (96%)	550 (98%)	12 (2%)	53	59
1	C	567/585 (97%)	558 (98%)	9 (2%)	62	69
1	D	563/585 (96%)	555 (99%)	8 (1%)	67	73
All	All	2259/2340 (96%)	2220 (98%)	39 (2%)	62	67

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	GLU
1	A	159	PHE
1	A	211	ASP
1	A	259	LYS
1	A	429	LYS
1	A	433	HIS
1	A	626[A]	VAL
1	A	626[B]	VAL
1	A	633	ARG
1	A	692	ASP
1	B	44	LYS
1	B	65	GLU
1	B	159	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	211	ASP
1	B	348	THR
1	B	433	HIS
1	B	451[A]	VAL
1	B	451[B]	VAL
1	B	471	LEU
1	B	554[A]	ARG
1	B	554[B]	ARG
1	B	592	LEU
1	C	65	GLU
1	C	159	PHE
1	C	211	ASP
1	C	388[A]	SER
1	C	388[B]	SER
1	C	429	LYS
1	C	441	LYS
1	C	626	VAL
1	C	638	LYS
1	D	65	GLU
1	D	159	PHE
1	D	211	ASP
1	D	261	LYS
1	D	398	ARG
1	D	433	HIS
1	D	441	LYS
1	D	591	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	C	422	GLN
1	D	175	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 40 ligands modelled in this entry, 4 are monoatomic - leaving 36 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	$\# Z > 2$
6	EDO	B	807	-	3,3,3	0.48	0	2,2,2	0.29	0
8	EOH	D	809	-	2,2,2	0.47	0	1,1,1	0.16	0
3	ACT	C	802	-	3,3,3	1.47	1 (33%)	3,3,3	1.29	0
6	EDO	C	810	-	3,3,3	0.44	0	2,2,2	0.38	0
8	EOH	B	810	-	2,2,2	0.47	0	1,1,1	0.19	0
8	EOH	D	810	-	2,2,2	0.46	0	1,1,1	0.11	0
5	PEG	A	805	-	6,6,6	0.48	0	5,5,5	0.55	0
4	PGE	D	804	-	9,9,9	0.36	0	8,8,8	0.25	0
9	1PE	B	804	-	15,15,15	0.51	0	14,14,14	0.49	0
2	HEM	D	801	7,1	41,50,50	1.48	5 (12%)	45,82,82	1.39	7 (15%)
3	ACT	A	803	-	3,3,3	1.51	1 (33%)	3,3,3	1.25	0
2	HEM	A	801	7,1	41,50,50	1.45	5 (12%)	45,82,82	1.40	6 (13%)
6	EDO	C	809	-	3,3,3	0.49	0	2,2,2	0.41	0
3	ACT	C	803	-	3,3,3	1.45	1 (33%)	3,3,3	1.44	0
4	PGE	A	804	-	9,9,9	0.33	0	8,8,8	0.30	0
3	ACT	B	803	-	3,3,3	1.23	0	3,3,3	1.31	0
8	EOH	A	809	-	2,2,2	0.46	0	1,1,1	0.06	0
3	ACT	D	803	-	3,3,3	1.43	1 (33%)	3,3,3	1.31	0
6	EDO	B	806	-	3,3,3	0.38	0	2,2,2	0.56	0
6	EDO	A	807	-	3,3,3	0.46	0	2,2,2	0.34	0
8	EOH	B	809	-	2,2,2	0.43	0	1,1,1	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PEG	C	807	-	6,6,6	0.52	0	5,5,5	0.46	0
4	PGE	B	805	-	9,9,9	0.30	0	8,8,8	0.33	0
6	EDO	D	807	-	3,3,3	0.48	0	2,2,2	0.30	0
2	HEM	B	801	7,1	41,50,50	1.47	5 (12%)	45,82,82	1.36	5 (11%)
3	ACT	A	802	-	3,3,3	1.39	0	3,3,3	1.45	0
5	PEG	C	806	-	6,6,6	0.50	0	5,5,5	0.40	0
6	EDO	A	806	-	3,3,3	0.49	0	2,2,2	0.30	0
6	EDO	C	808	-	3,3,3	0.44	0	2,2,2	0.41	0
2	HEM	C	801	7,1	41,50,50	1.45	3 (7%)	45,82,82	1.41	6 (13%)
6	EDO	D	805	-	3,3,3	0.50	0	2,2,2	0.33	0
3	ACT	B	802	-	3,3,3	1.45	0	3,3,3	1.29	0
3	ACT	D	802	-	3,3,3	1.29	0	3,3,3	1.50	0
6	EDO	D	806	-	3,3,3	0.46	0	2,2,2	0.40	0
5	PEG	C	805	-	6,6,6	0.48	0	5,5,5	0.57	0
10	PG4	C	804	-	12,12,12	0.51	0	11,11,11	0.34	0

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
6	EDO	B	807	-	-	0/1/1/1	-
6	EDO	C	810	-	-	1/1/1/1	-
5	PEG	A	805	-	-	4/4/4/4	-
4	PGE	D	804	-	-	4/7/7/7	-
9	1PE	B	804	-	-	8/13/13/13	-
2	HEM	D	801	7,1	-	2/12/54/54	-
2	HEM	A	801	7,1	-	2/12/54/54	-
6	EDO	C	809	-	-	1/1/1/1	-
4	PGE	A	804	-	-	6/7/7/7	-
6	EDO	B	806	-	-	0/1/1/1	-
6	EDO	A	807	-	-	1/1/1/1	-
5	PEG	C	807	-	-	1/4/4/4	-
4	PGE	B	805	-	-	3/7/7/7	-
6	EDO	D	807	-	-	0/1/1/1	-
2	HEM	B	801	7,1	-	4/12/54/54	-
5	PEG	C	806	-	-	2/4/4/4	-
6	EDO	A	806	-	-	0/1/1/1	-
6	EDO	C	808	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	801	7,1	-	3/12/54/54	-
6	EDO	D	805	-	-	0/1/1/1	-
6	EDO	D	806	-	-	1/1/1/1	-
5	PEG	C	805	-	-	1/4/4/4	-
10	PG4	C	804	-	-	4/10/10/10	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	HEM	C3C-C2C	-3.87	1.35	1.40
2	B	801	HEM	C3C-C2C	-3.83	1.35	1.40
2	A	801	HEM	C3C-C2C	-3.79	1.35	1.40
2	B	801	HEM	C3C-CAC	3.79	1.55	1.47
2	D	801	HEM	C3C-C2C	-3.79	1.35	1.40
2	C	801	HEM	C3C-CAC	3.78	1.55	1.47
2	D	801	HEM	C3C-CAC	3.70	1.55	1.47
2	A	801	HEM	C3C-CAC	3.69	1.55	1.47
2	B	801	HEM	CAB-C3B	3.01	1.55	1.47
2	C	801	HEM	CAB-C3B	3.00	1.55	1.47
2	D	801	HEM	CAB-C3B	3.00	1.55	1.47
2	A	801	HEM	CAB-C3B	2.86	1.55	1.47
2	D	801	HEM	CMB-C2B	2.22	1.55	1.50
3	A	803	ACT	CH3-C	2.21	1.58	1.49
3	C	802	ACT	CH3-C	2.21	1.58	1.49
2	B	801	HEM	CMB-C2B	2.19	1.55	1.50
2	A	801	HEM	FE-ND	2.11	2.07	1.96
3	D	803	ACT	CH3-C	2.11	1.57	1.49
3	C	803	ACT	CH3-C	2.10	1.57	1.49
2	A	801	HEM	CMB-C2B	2.10	1.55	1.50
2	D	801	HEM	FE-ND	2.05	2.07	1.96
2	B	801	HEM	CAA-C2A	2.01	1.55	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	HEM	C4D-ND-C1D	3.26	108.44	105.07
2	C	801	HEM	C4D-ND-C1D	3.18	108.36	105.07
2	B	801	HEM	C1B-NB-C4B	3.11	108.28	105.07
2	A	801	HEM	C1B-NB-C4B	3.07	108.25	105.07
2	B	801	HEM	C4D-ND-C1D	2.99	108.16	105.07
2	A	801	HEM	C4D-ND-C1D	2.97	108.14	105.07
2	D	801	HEM	C1B-NB-C4B	2.90	108.07	105.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	HEM	CAA-CBA-CGA	-2.71	106.16	113.76
2	B	801	HEM	C4C-CHD-C1D	2.64	126.05	122.56
2	C	801	HEM	C4C-CHD-C1D	2.61	126.01	122.56
2	A	801	HEM	CAA-CBA-CGA	-2.57	106.55	113.76
2	C	801	HEM	C1B-NB-C4B	2.50	107.66	105.07
2	B	801	HEM	CAA-CBA-CGA	-2.40	107.03	113.76
2	C	801	HEM	CMC-C2C-C3C	2.40	129.16	124.68
2	A	801	HEM	C4C-CHD-C1D	2.37	125.68	122.56
2	D	801	HEM	C3D-C4D-ND	-2.30	107.61	110.17
2	D	801	HEM	C4A-C3A-C2A	2.29	108.59	107.00
2	C	801	HEM	C3D-C4D-ND	-2.27	107.64	110.17
2	A	801	HEM	C3D-C4D-ND	-2.25	107.66	110.17
2	D	801	HEM	CAA-CBA-CGA	-2.17	107.67	113.76
2	D	801	HEM	C4C-CHD-C1D	2.13	125.37	122.56
2	A	801	HEM	CMC-C2C-C3C	2.04	128.50	124.68
2	D	801	HEM	C2D-C1D-ND	-2.02	107.46	109.88
2	B	801	HEM	C3D-C4D-ND	-2.02	107.92	110.17

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	804	PGE	C4-C3-O2-C2
4	A	804	PGE	O2-C3-C4-O3
9	B	804	1PE	OH6-C15-C25-OH5
4	D	804	PGE	O3-C5-C6-O4
5	A	805	PEG	O2-C3-C4-O4
5	C	806	PEG	O2-C3-C4-O4
10	C	804	PG4	C5-C6-O4-C7
4	D	804	PGE	O1-C1-C2-O2
5	A	805	PEG	O1-C1-C2-O2
9	B	804	1PE	OH2-C12-C22-OH3
4	A	804	PGE	O1-C1-C2-O2
6	C	809	EDO	O1-C1-C2-O2
6	D	806	EDO	O1-C1-C2-O2
4	B	805	PGE	O3-C5-C6-O4
9	B	804	1PE	OH7-C16-C26-OH6
4	B	805	PGE	O2-C3-C4-O3
5	A	805	PEG	C4-C3-O2-C2
4	B	805	PGE	C1-C2-O2-C3
5	C	807	PEG	C4-C3-O2-C2
5	C	806	PEG	C4-C3-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	804	PGE	C3-C4-O3-C5
10	C	804	PG4	O4-C7-C8-O5
9	B	804	1PE	C25-C15-OH6-C26
9	B	804	1PE	C13-C23-OH3-C22
5	C	805	PEG	C1-C2-O2-C3
10	C	804	PG4	C3-C4-O3-C5
4	A	804	PGE	C1-C2-O2-C3
6	A	807	EDO	O1-C1-C2-O2
2	B	801	HEM	CAA-CBA-CGA-O1A
2	C	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O1A
9	B	804	1PE	C12-C22-OH3-C23
2	D	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	CAD-CBD-CGD-O2D
2	C	801	HEM	CAA-CBA-CGA-O2A
2	D	801	HEM	CAA-CBA-CGA-O2A
9	B	804	1PE	C14-C24-OH4-C13
2	B	801	HEM	CAD-CBD-CGD-O1D
5	A	805	PEG	C1-C2-O2-C3
4	D	804	PGE	O2-C3-C4-O3
10	C	804	PG4	O2-C3-C4-O3
6	C	810	EDO	O1-C1-C2-O2
4	A	804	PGE	C3-C4-O3-C5
4	A	804	PGE	C6-C5-O3-C4
2	C	801	HEM	CAD-CBD-CGD-O2D
9	B	804	1PE	OH4-C13-C23-OH3

There are no ring outliers.

14 monomers are involved in 18 short contacts:

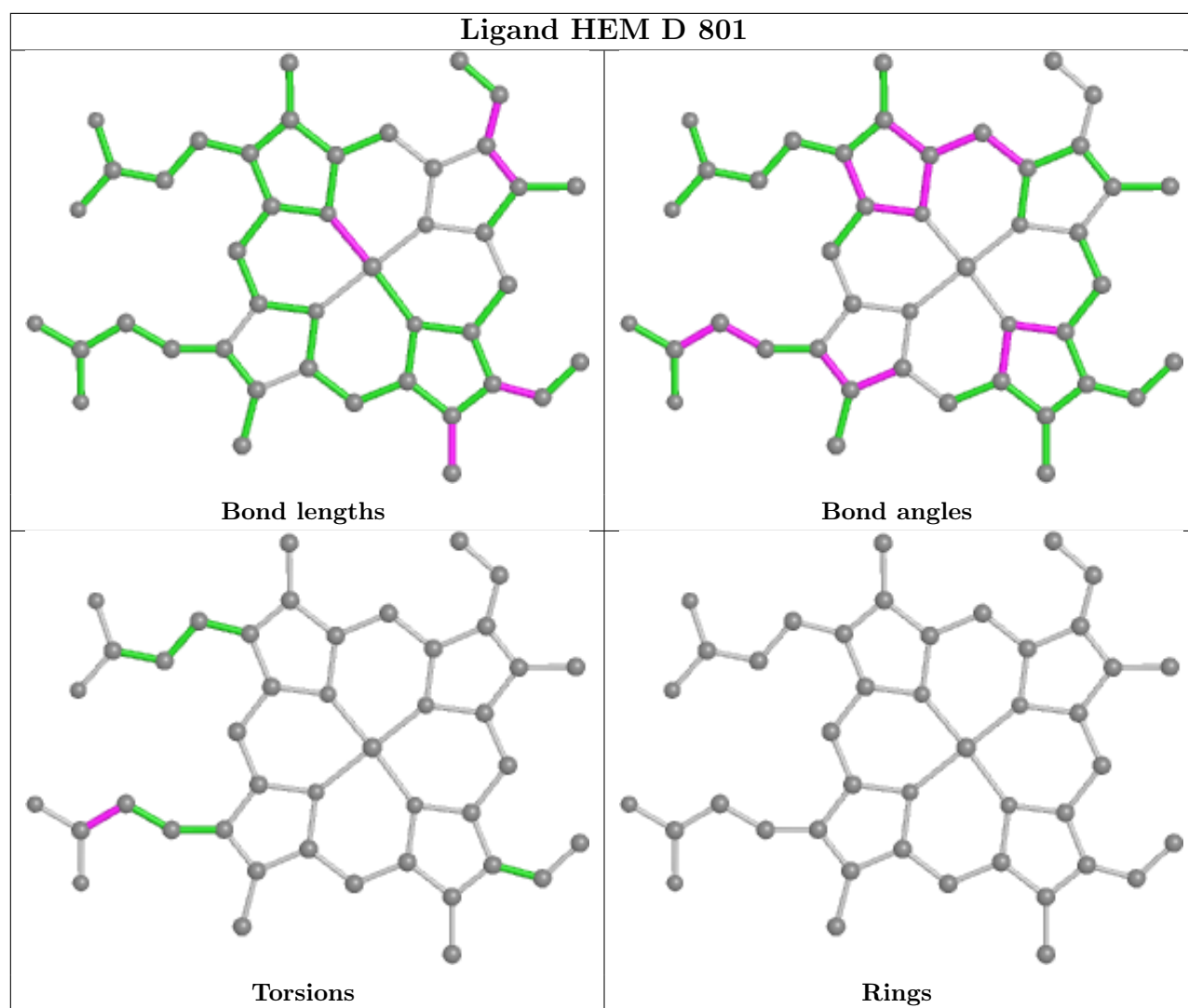
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	809	EOH	2	0
3	C	802	ACT	1	0
4	D	804	PGE	1	0
9	B	804	1PE	1	0
2	D	801	HEM	1	0
2	A	801	HEM	1	0
3	C	803	ACT	1	0
6	A	807	EDO	1	0
4	B	805	PGE	1	0

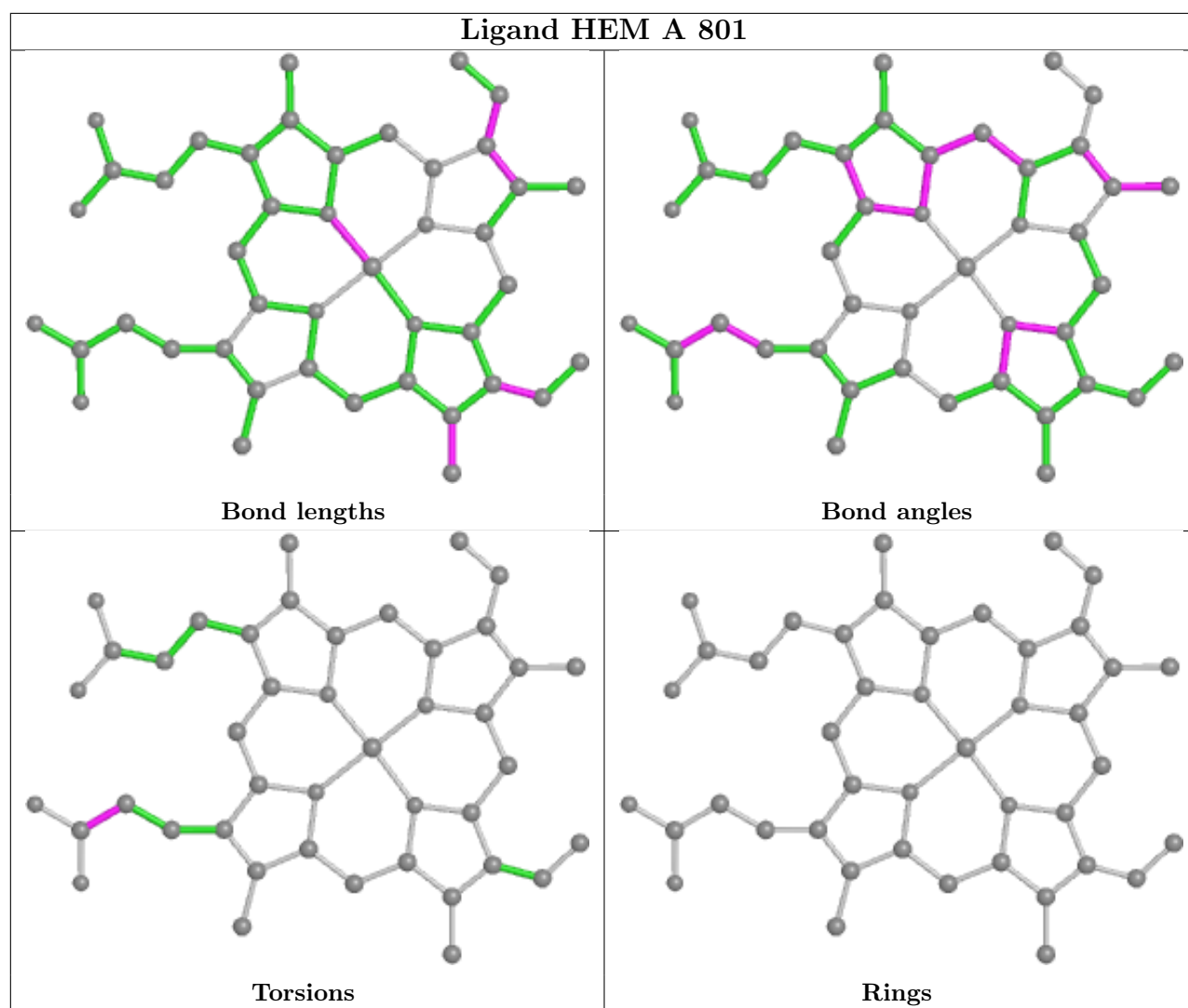
Continued on next page...

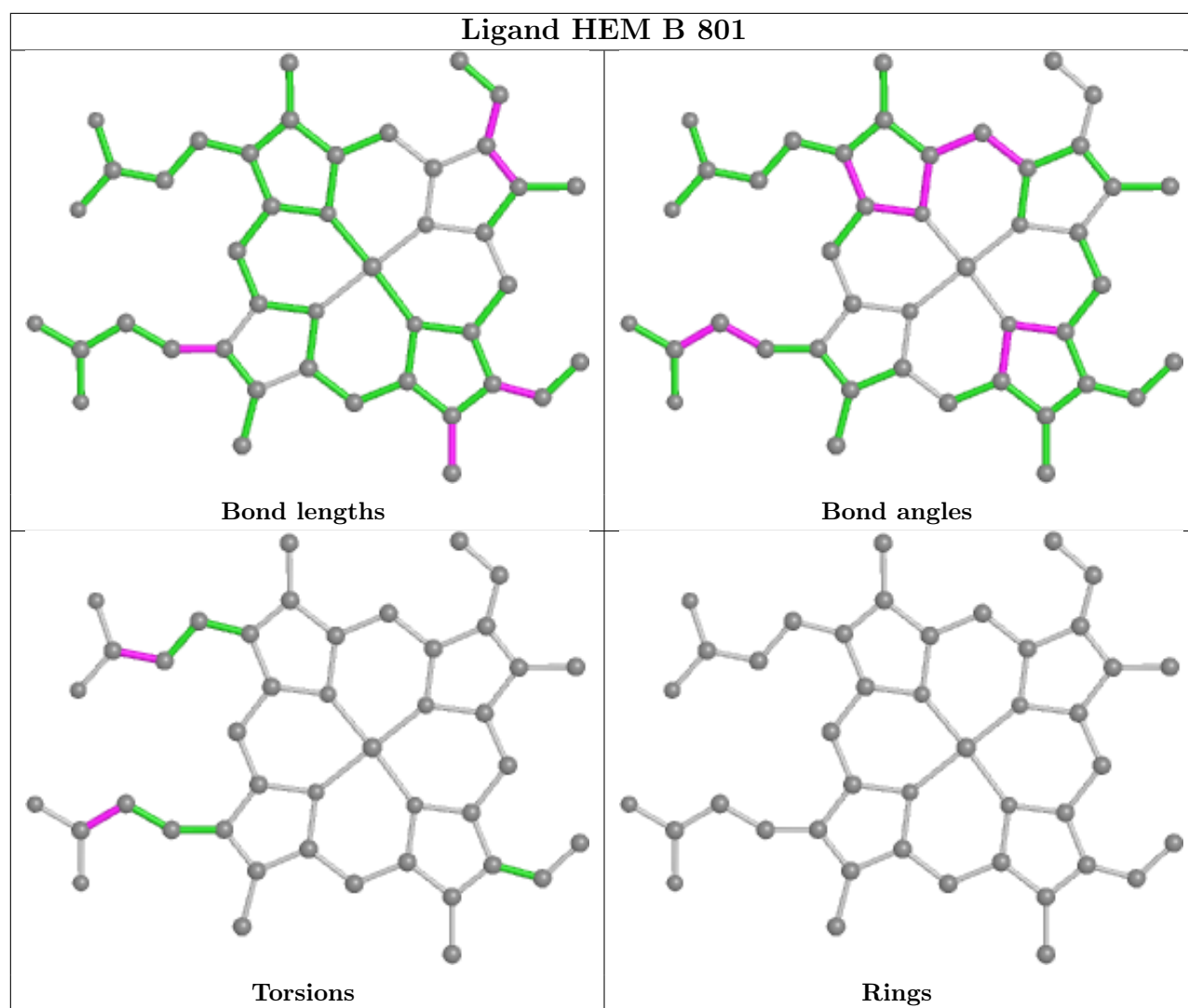
Continued from previous page...

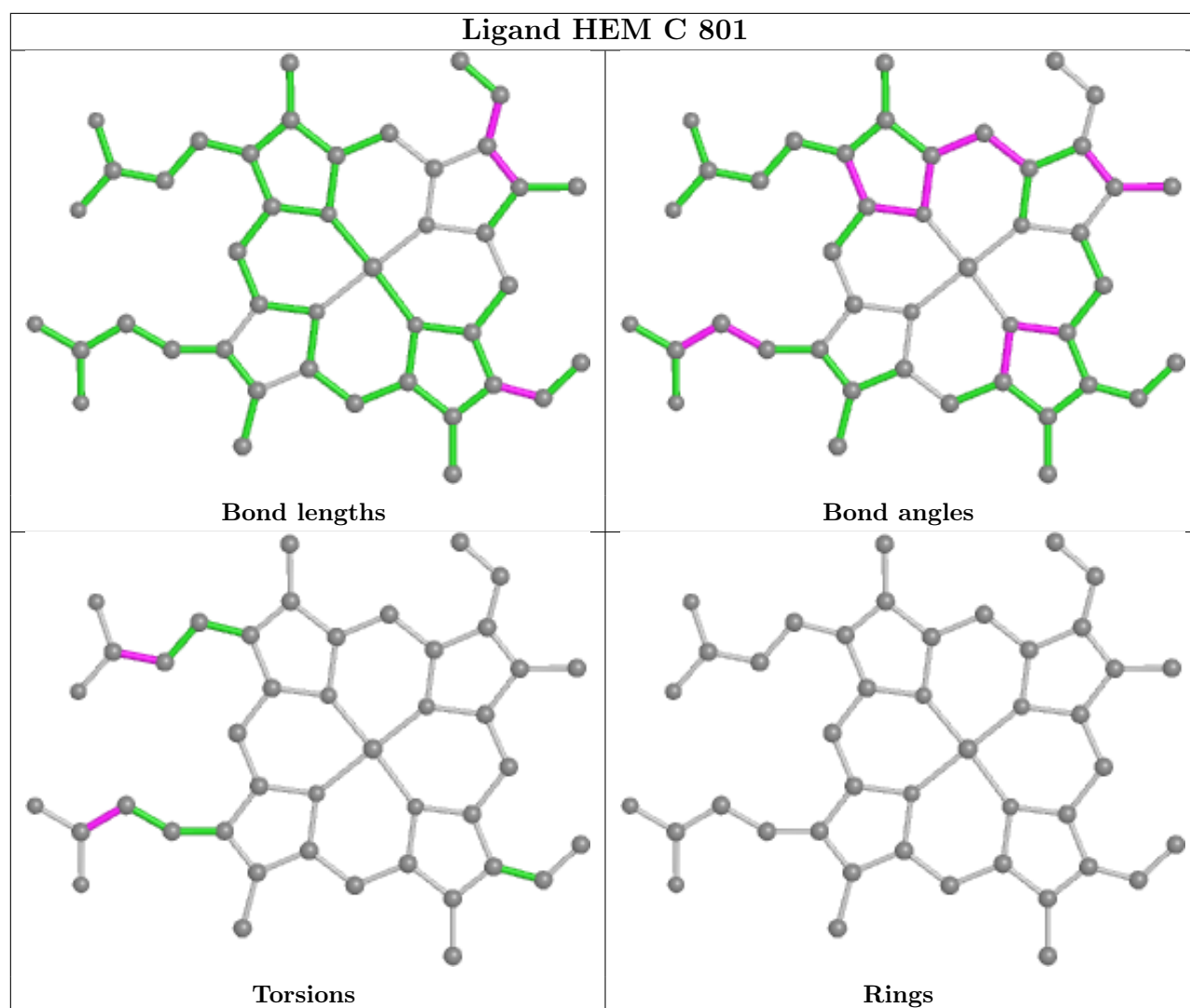
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	807	EDO	1	0
6	C	808	EDO	1	0
2	C	801	HEM	1	0
3	D	802	ACT	1	0
10	C	804	PG4	4	0

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.









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	682/719 (94%)	-0.37	9 (1%) 77 80	9, 17, 37, 76	0
1	B	677/719 (94%)	-0.45	3 (0%) 92 93	7, 15, 33, 55	0
1	C	679/719 (94%)	-0.45	5 (0%) 87 89	7, 15, 33, 56	0
1	D	677/719 (94%)	-0.39	8 (1%) 79 82	8, 17, 35, 68	0
All	All	2715/2876 (94%)	-0.42	25 (0%) 84 86	7, 16, 34, 76	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	718	GLU	4.9
1	D	641	MET	4.1
1	D	637	GLY	3.9
1	D	682	LYS	3.8
1	A	637	GLY	3.8
1	D	680	GLU	3.8
1	A	638	LYS	3.6
1	D	715	GLY	3.1
1	C	716	ASP	3.1
1	C	715	GLY	3.0
1	C	637	GLY	2.9
1	B	637	GLY	2.9
1	A	719	GLU	2.9
1	D	681	GLU	2.9
1	B	682	LYS	2.8
1	A	682	LYS	2.5
1	C	638	LYS	2.5
1	A	41	GLN	2.5
1	A	579	GLY	2.4
1	B	638	LYS	2.3
1	A	257	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	636	SER	2.1
1	C	451	VAL	2.1
1	A	715	GLY	2.1
1	D	638	LYS	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 monosaccharides 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(\AA^2)	Q<0.9
3	ACT	D	803	4/4	0.81	0.18	19,22,22,26	0
8	EOH	B	810	3/3	0.82	0.26	26,26,28,30	0
4	PGE	D	804	10/10	0.83	0.18	24,26,27,28	0
6	EDO	D	805	4/4	0.85	0.16	25,25,27,28	0
6	EDO	C	809	4/4	0.86	0.14	24,25,26,28	0
3	ACT	A	803	4/4	0.87	0.17	23,23,25,31	0
8	EOH	D	809	3/3	0.87	0.18	24,24,26,32	0
8	EOH	B	809	3/3	0.88	0.13	22,22,23,27	0
3	ACT	C	803	4/4	0.88	0.15	19,20,20,22	0
6	EDO	C	808	4/4	0.88	0.23	26,27,27,31	0
7	O	D	808	1/1	0.89	0.30	12,12,12,12	1
3	ACT	B	803	4/4	0.89	0.14	14,15,16,17	0
9	1PE	B	804	16/16	0.89	0.15	24,26,29,30	0
8	EOH	A	809	3/3	0.90	0.13	21,21,22,25	0
5	PEG	C	806	7/7	0.90	0.12	21,24,25,25	0
6	EDO	A	807	4/4	0.90	0.17	24,25,27,31	0
6	EDO	D	806	4/4	0.90	0.23	24,27,28,29	0
4	PGE	A	804	10/10	0.90	0.18	22,24,26,28	0
10	PG4	C	804	13/13	0.91	0.16	23,24,26,26	0

Continued on next page...

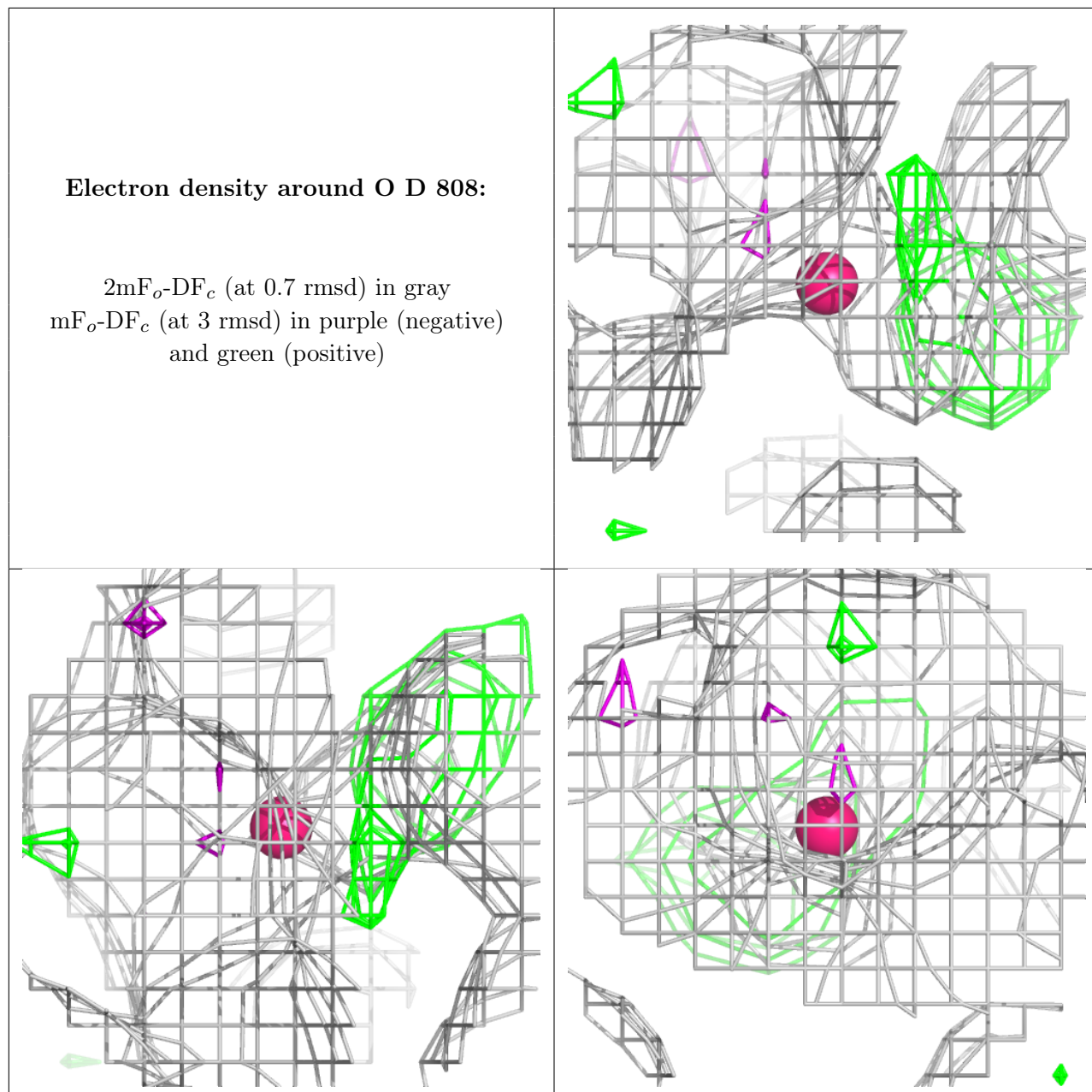
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	EDO	B	807	4/4	0.92	0.20	29,30,31,31	0
8	EOH	D	810	3/3	0.93	0.18	22,22,23,25	0
6	EDO	D	807	4/4	0.93	0.19	24,25,25,27	0
5	PEG	C	807	7/7	0.93	0.19	23,24,25,26	0
7	O	B	808	1/1	0.94	0.18	11,11,11,11	1
5	PEG	C	805	7/7	0.94	0.24	25,26,28,29	0
4	PGE	B	805	10/10	0.94	0.12	21,24,27,28	0
6	EDO	B	806	4/4	0.95	0.20	23,23,25,26	0
6	EDO	A	806	4/4	0.96	0.14	25,25,26,27	0
5	PEG	A	805	7/7	0.96	0.19	23,24,25,27	0
6	EDO	C	810	4/4	0.96	0.11	25,26,27,28	0
2	HEM	B	801	43/43	0.97	0.09	4,10,15,18	0
2	HEM	A	801	43/43	0.97	0.10	4,9,14,20	0
3	ACT	B	802	4/4	0.97	0.09	11,11,12,13	0
7	O	C	811	1/1	0.97	0.13	11,11,11,11	1
2	HEM	D	801	43/43	0.98	0.08	5,10,16,22	0
3	ACT	A	802	4/4	0.98	0.10	12,13,14,14	0
2	HEM	C	801	43/43	0.98	0.09	4,10,14,16	0
3	ACT	D	802	4/4	0.98	0.10	16,17,17,19	0
3	ACT	C	802	4/4	0.99	0.06	16,17,17,18	0
7	O	A	808	1/1	0.99	0.10	13,13,13,13	1

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.

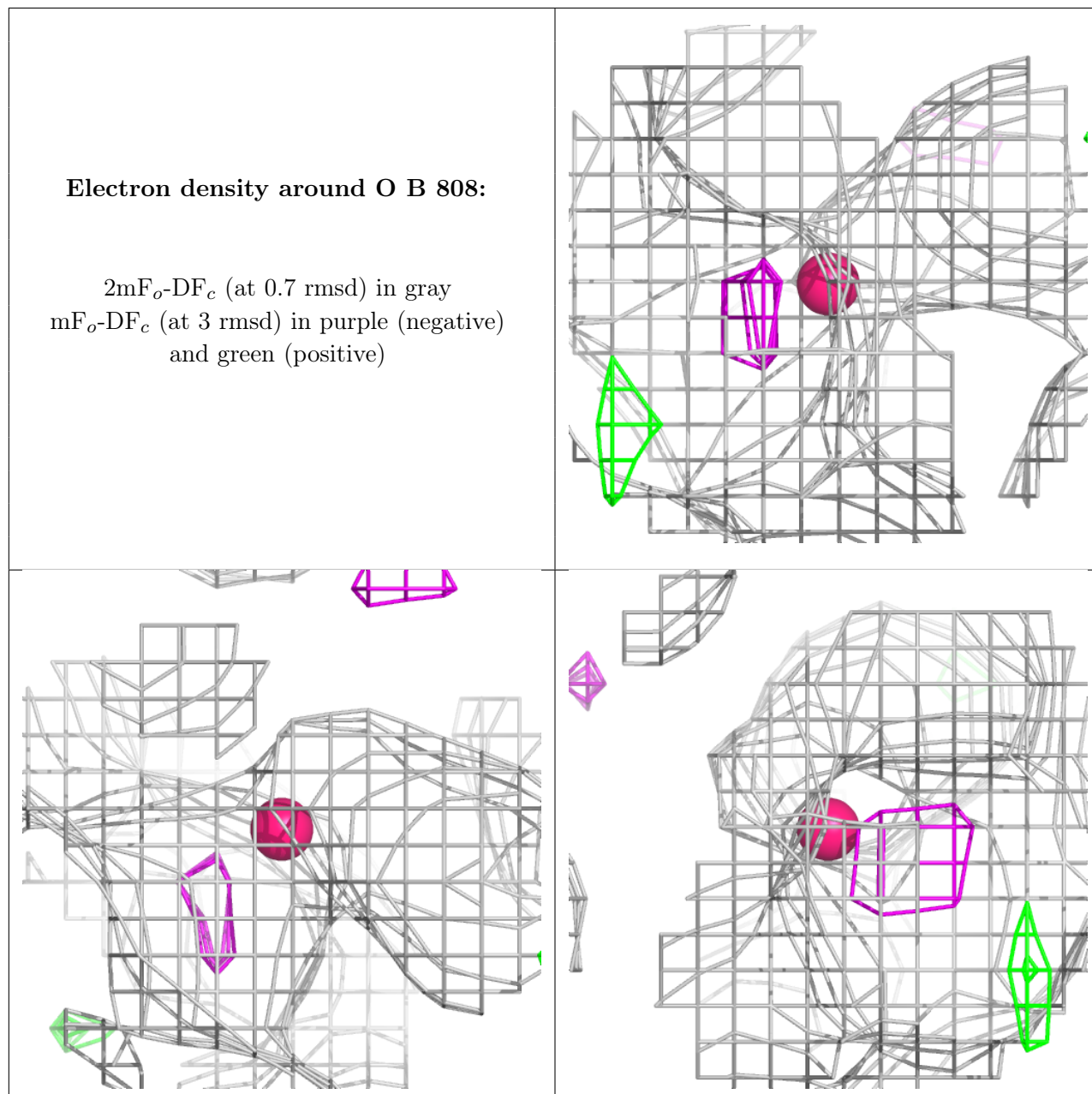
Electron density around O D 808:

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



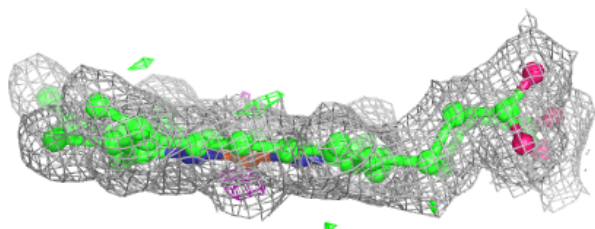
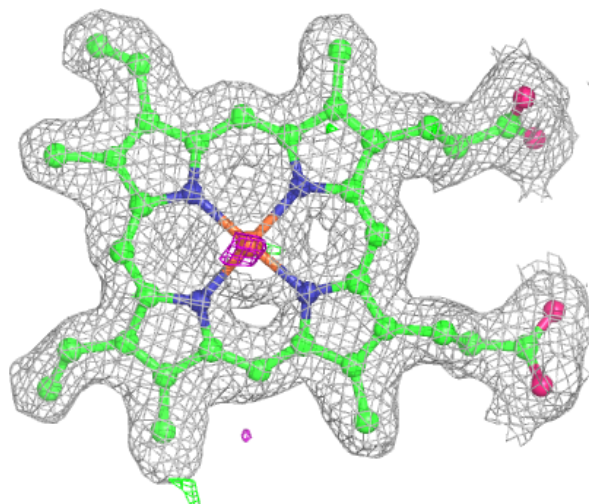
Electron density around O B 808:

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



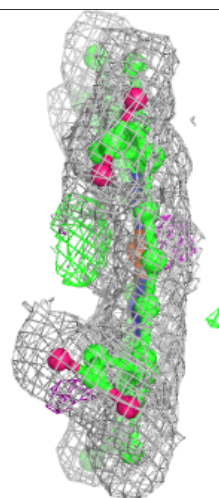
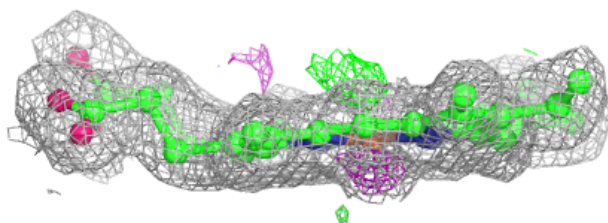
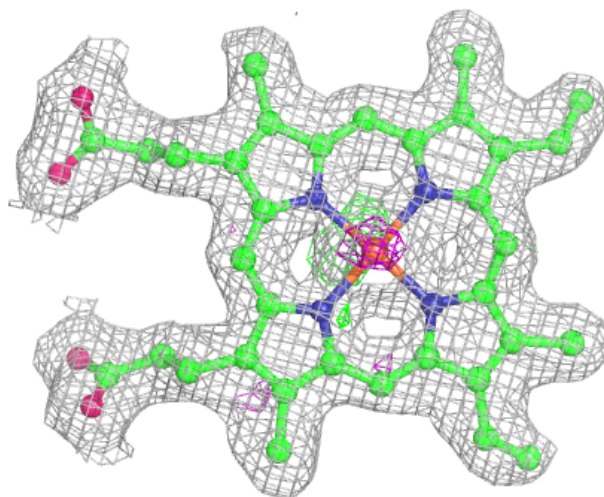
Electron density around HEM B 801:

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



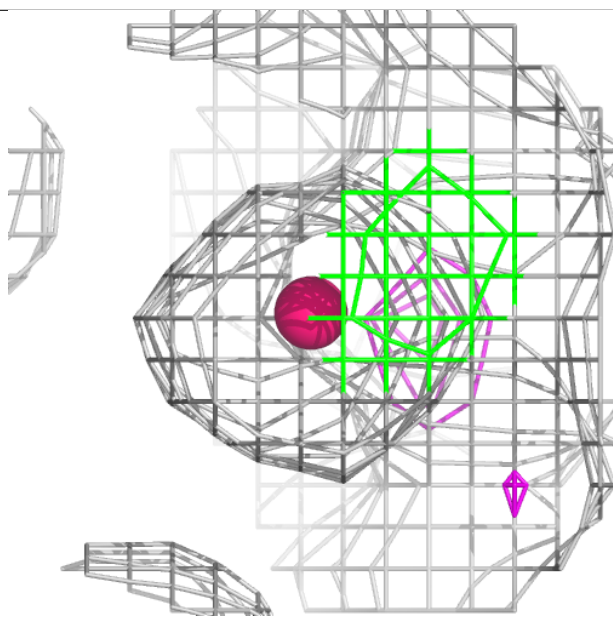
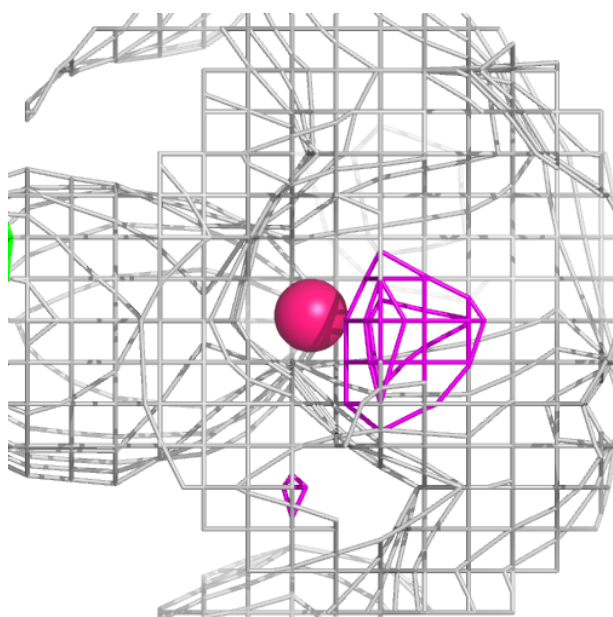
Electron density around HEM A 801:

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



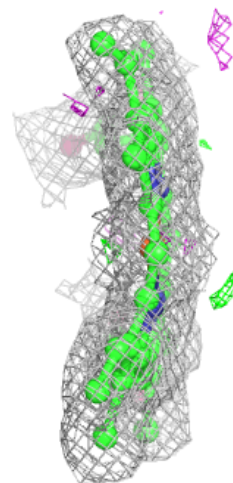
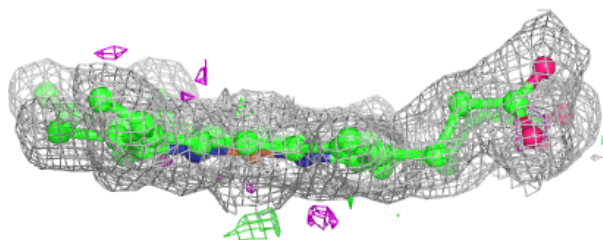
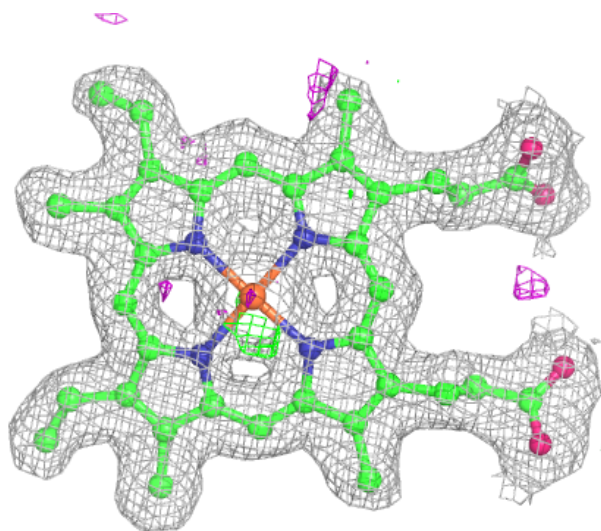
Electron density around O C 811:

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



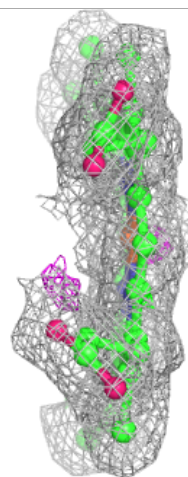
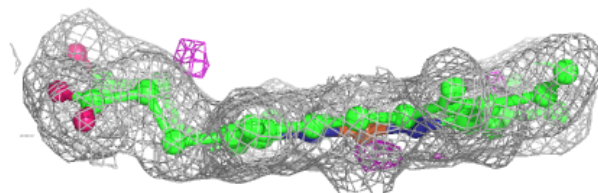
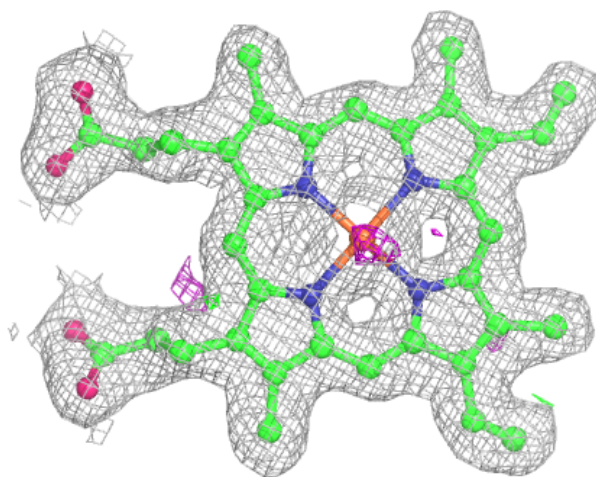
Electron density around HEM D 801:

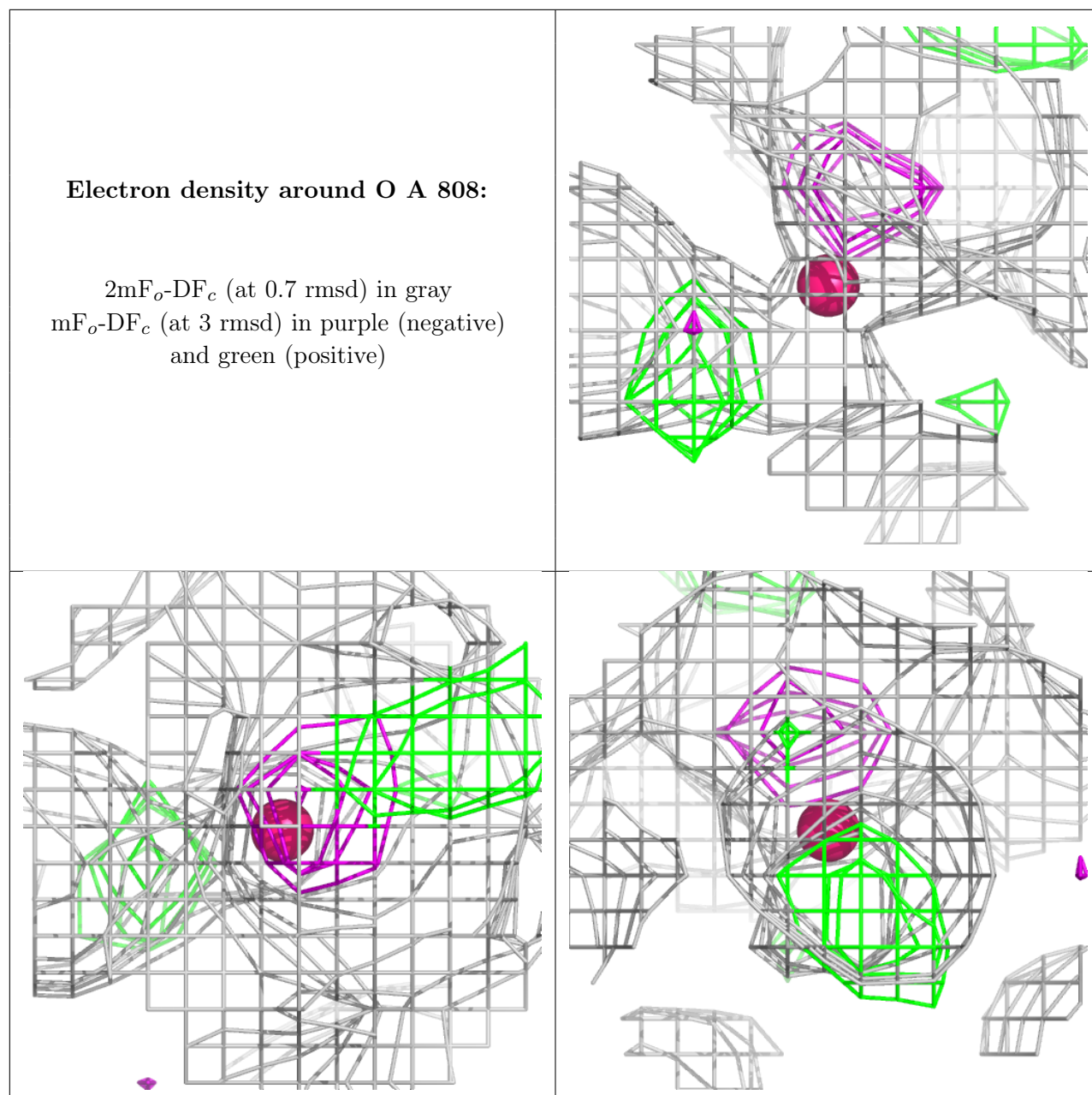
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 801:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.