



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:53 PM UTC

PDB ID : 6ZTX / pdb_00006ztx
Title : Crystal Structure of catalase HP11 from Escherichia coli (serendipitously crystallized)
Authors : Grzechowiak, M.; Sekula, B.; Ruszkowski, M.
Deposited on : 2020-07-20
Resolution : 1.30 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	:	2022.3.0, CSD as543be (2022)
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

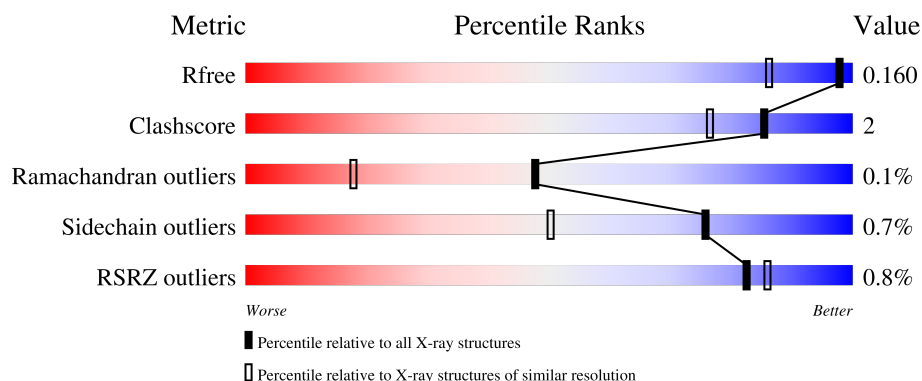
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

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	753	% 92% 5% .
1	B	753	% 91% 5% .
1	C	753	% 91% 6% .
1	D	753	% 91% 5% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26887 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 Catalase HPIL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	18	0
			5866	3723	1019	1109	15			
1	B	727	Total	C	N	O	S	0	12	0
			5826	3696	1015	1102	13			
1	C	727	Total	C	N	O	S	0	12	0
			5826	3696	1013	1103	14			
1	D	727	Total	C	N	O	S	0	13	0
			5832	3698	1016	1104	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	SER	ARG	variant	UNP P21179
A	99	ASP	SER	variant	UNP P21179
A	372	ASN	LYS	variant	UNP P21179
A	521	SER	ARG	variant	UNP P21179
B	37	SER	ARG	variant	UNP P21179
B	99	ASP	SER	variant	UNP P21179
B	372	ASN	LYS	variant	UNP P21179
B	521	SER	ARG	variant	UNP P21179
C	37	SER	ARG	variant	UNP P21179
C	99	ASP	SER	variant	UNP P21179
C	372	ASN	LYS	variant	UNP P21179
C	521	SER	ARG	variant	UNP P21179
D	37	SER	ARG	variant	UNP P21179
D	99	ASP	SER	variant	UNP P21179
D	372	ASN	LYS	variant	UNP P21179
D	521	SER	ARG	variant	UNP P21179

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



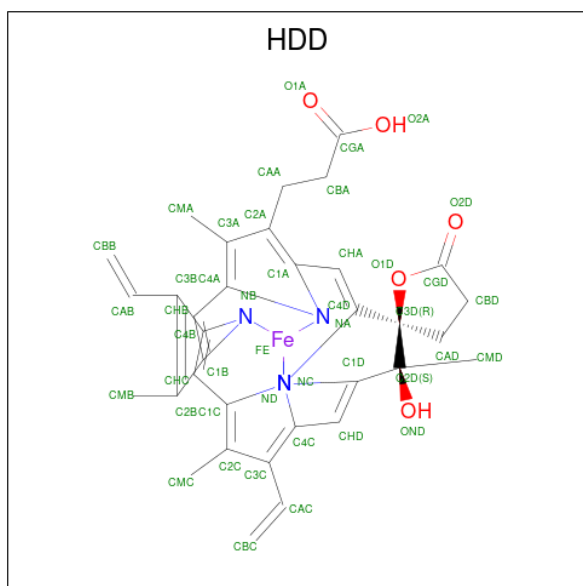
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: HDD) (formula: $C_{34}H_{32}FeN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
4	B	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
4	C	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
4	D	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		

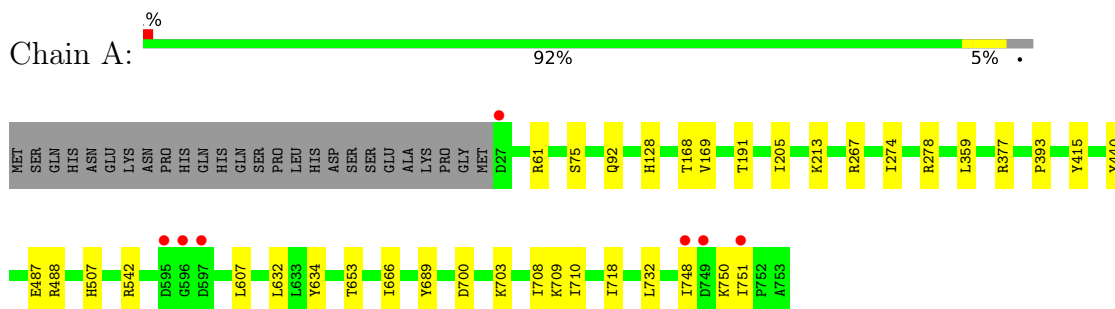
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	867	Total 867	O 867	0	0
5	B	780	Total 780	O 780	0	0
5	C	784	Total 784	O 784	0	0
5	D	878	Total 878	O 878	0	0

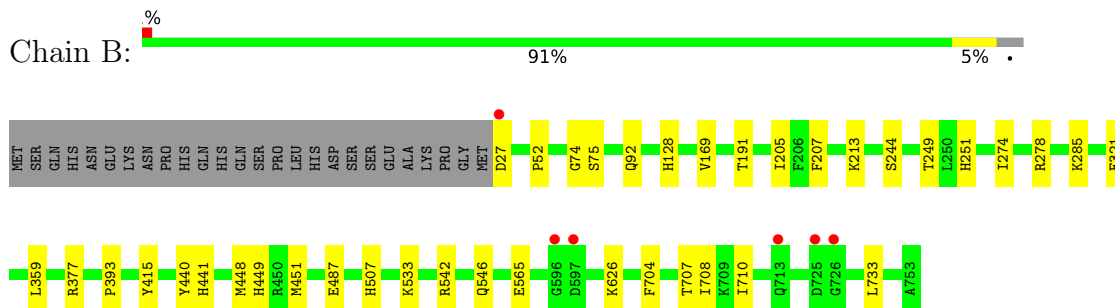
3 Residue-property plots

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.

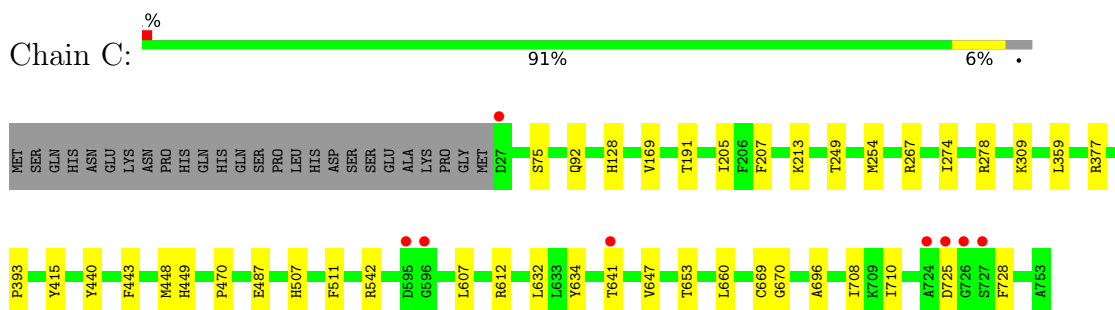
• Molecule 1: Catalase HP1I



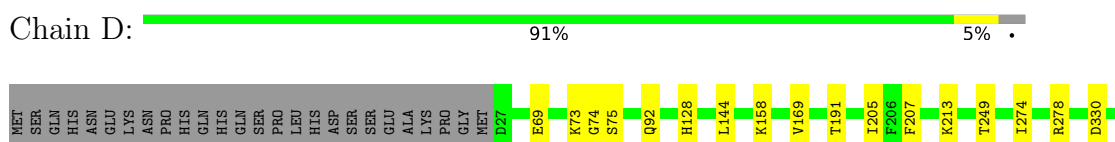
• Molecule 1: Catalase HP1I

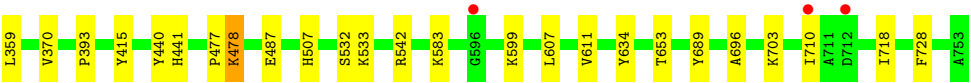


• Molecule 1: Catalase HP1I



• Molecule 1: Catalase HP1I





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.21Å 132.93Å 121.65Å 90.00° 109.65° 90.00°	Depositor
Resolution (Å)	44.76 – 1.30 44.76 – 1.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (44.76-1.30) 98.0 (44.76-1.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.30Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.135 , 0.162 0.134 , 0.160	Depositor DCC
R_{free} test set	1342 reflections (0.20%)	wwPDB-VP
Wilson B-factor (Å ²)	11.4	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	26887	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: EDO, HDD, GOL

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	0.23	0/6048	0.48	0/8220
1	B	0.22	0/5999	0.46	0/8156
1	C	0.22	0/5996	0.46	0/8152
1	D	0.23	0/6001	0.48	0/8157
All	All	0.23	0/24044	0.47	0/32685

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	5866	0	5689	23	0
1	B	5826	0	5642	25	0
1	C	5826	0	5637	23	0
1	D	5832	0	5648	31	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
3	A	8	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8	0	12	4	0
3	C	4	0	6	1	0
3	D	8	0	12	2	0
4	A	44	0	31	2	0
4	B	44	0	31	2	0
4	C	44	0	31	2	0
4	D	44	0	31	2	0
5	A	867	0	0	4	0
5	B	780	0	0	4	0
5	C	784	0	0	2	0
5	D	878	0	0	9	0
All	All	26887	0	22814	101	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 2.

All (101) 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:542:ARG:HH21	3:A:803:EDO:H22	1.45	0.80
1:C:542:ARG:HH21	3:C:802:EDO:H22	1.47	0.79
1:D:542:ARG:HH21	3:D:1201:EDO:H11	1.48	0.78
1:B:542:ARG:HH21	3:B:803:EDO:H22	1.49	0.75
1:A:267[B]:ARG:NH1	5:A:902:HOH:O	2.25	0.69
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.75	0.68
1:A:666:ILE:HD11	1:A:732:LEU:HD22	1.79	0.64
1:D:74:GLY:H	3:D:1203:EDO:H11	1.63	0.63
1:B:27:ASP:N	5:B:904:HOH:O	2.33	0.62
1:D:689:TYR:CE1	1:D:710:ILE:HD11	2.36	0.61
1:A:708:ILE:HG13	1:A:710:ILE:HG13	1.84	0.60
1:B:74:GLY:H	3:B:802:EDO:H11	1.67	0.60
1:A:710:ILE:CD1	1:A:718:ILE:HG13	2.32	0.60
1:D:533:LYS:HE3	5:D:1301:HOH:O	2.01	0.60
1:A:61:ARG:NH2	5:A:908:HOH:O	2.34	0.59
1:B:708:ILE:HG13	1:B:710:ILE:HG12	1.84	0.58
1:C:254[B]:MET:HG2	1:C:511:PHE:CD2	2.40	0.57
1:C:612:ARG:NH1	5:C:907:HOH:O	2.34	0.56
1:D:710:ILE:CD1	1:D:718:ILE:HG13	2.36	0.55
1:A:689:TYR:CE1	1:A:710:ILE:HD11	2.41	0.55
1:B:533:LYS:NZ	5:B:908:HOH:O	2.40	0.54
1:B:359:LEU:H	1:B:507:HIS:HD2	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254[B]:MET:HG2	1:C:511:PHE:HD2	1.72	0.53
1:C:725:ASP:H	1:C:728:PHE:HB3	1.74	0.53
1:B:213:LYS:HD3	1:C:92:GLN:HA	1.91	0.52
1:B:285:LYS:NZ	5:B:910:HOH:O	2.42	0.52
1:D:359:LEU:H	1:D:507:HIS:HD2	1.57	0.51
1:A:92:GLN:HA	1:D:213:LYS:HD3	1.93	0.51
1:B:274:ILE:HD12	4:B:804:HDD:HMB3	1.93	0.51
1:C:359:LEU:H	1:C:507:HIS:HD2	1.59	0.50
1:B:626:LYS:HG3	1:B:733:LEU:HD13	1.93	0.50
1:A:128:HIS:CE1	1:A:169:VAL:HG22	2.48	0.49
1:D:144:LEU:HD11	1:D:370:VAL:HG13	1.95	0.49
1:D:689:TYR:HE1	1:D:710:ILE:HD11	1.78	0.49
1:D:710:ILE:HD13	1:D:718:ILE:HG13	1.95	0.48
1:A:359:LEU:H	1:A:507:HIS:HD2	1.61	0.48
1:B:321[A]:GLU:HG2	5:B:1457:HOH:O	2.14	0.48
1:C:267:ARG:NH1	5:C:910:HOH:O	2.39	0.48
1:A:278:ARG:HH22	1:A:487[B]:GLU:CD	2.22	0.47
1:C:278:ARG:HH22	1:C:487[B]:GLU:CD	2.21	0.47
1:D:158:LYS:HB3	5:D:1391:HOH:O	2.13	0.47
1:A:213:LYS:HD3	1:D:92:GLN:HA	1.96	0.47
1:A:710:ILE:HD12	1:A:718:ILE:HG13	1.97	0.47
1:A:750:LYS:NZ	5:A:919:HOH:O	2.47	0.47
1:B:92:GLN:HA	1:C:213:LYS:HD3	1.97	0.47
1:C:274:ILE:HD12	4:C:803:HDD:HMB3	1.97	0.47
1:D:278:ARG:HH22	1:D:487[B]:GLU:CD	2.23	0.47
1:B:448:MET:HG3	1:B:449[A]:HIS:CD2	2.50	0.46
1:A:700:ASP:HB3	1:A:703:LYS:HE2	1.98	0.46
1:A:488:ARG:NH1	5:A:906:HOH:O	2.29	0.46
1:C:128:HIS:CE1	1:C:169:VAL:HG22	2.50	0.46
1:A:709:LYS:HA	1:A:709:LYS:HD3	1.84	0.46
1:C:448:MET:HG3	1:C:449[A]:HIS:CD2	2.50	0.46
1:D:274:ILE:HD12	4:D:1204:HDD:HMB3	1.98	0.45
1:C:607:LEU:HD11	1:C:632:LEU:HB3	1.98	0.45
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.51	0.45
1:C:393:PRO:HD2	1:C:415:TYR:CG	2.52	0.45
1:D:69:GLU:HG3	5:D:2005:HOH:O	2.17	0.45
4:C:803:HDD:HAD2	4:C:803:HDD:HMD3	1.61	0.45
1:D:607:LEU:HD22	1:D:611:VAL:HG21	1.97	0.45
1:A:274:ILE:HD12	4:A:804:HDD:HMB3	1.99	0.44
1:B:278:ARG:HH22	1:B:487:GLU:CD	2.25	0.44
1:D:477:PRO:C	1:D:478:LYS:HG2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.51	0.44
1:D:703:LYS:HA	1:D:703:LYS:HD3	1.88	0.44
1:C:309:LYS:HD2	1:C:660:LEU:HD11	1.99	0.43
1:D:393:PRO:HD2	1:D:415:TYR:CG	2.54	0.43
1:B:128:HIS:CE1	1:B:169:VAL:HG22	2.54	0.43
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.53	0.43
1:B:704:PHE:O	1:B:707:THR:HG22	2.18	0.43
1:D:634:TYR:O	1:D:653:THR:HA	2.18	0.43
1:C:641:THR:HG22	1:C:647:VAL:HG22	2.01	0.42
1:A:393:PRO:HD2	1:A:415:TYR:CG	2.54	0.42
1:B:244:SER:HA	1:B:546[B]:GLN:OE1	2.19	0.42
1:B:441:HIS:CD2	1:D:73[A]:LYS:HD2	2.55	0.42
3:B:802:EDO:H12	1:D:441:HIS:NE2	2.35	0.42
1:C:696:ALA:HB1	1:C:728:PHE:CZ	2.54	0.42
1:D:583:LYS:HG2	5:D:1846:HOH:O	2.19	0.42
4:D:1204:HDD:HBD2	5:D:1636:HOH:O	2.18	0.42
1:A:607:LEU:HD11	1:A:632:LEU:HB3	2.02	0.42
1:C:669:CYS:SG	1:C:670:GLY:N	2.91	0.42
1:D:532[A]:SER:OG	5:D:1301:HOH:O	2.21	0.42
1:B:52:PRO:HG3	5:D:1722:HOH:O	2.19	0.42
1:A:748[A]:ILE:O	1:A:751:ILE:HG22	2.19	0.42
1:C:207:PHE:O	1:C:249:THR:HA	2.19	0.42
1:D:207:PHE:O	1:D:249:THR:HA	2.20	0.42
1:D:330[B]:ASP:OD1	5:D:1302:HOH:O	2.22	0.42
1:B:74:GLY:H	3:B:802:EDO:C1	2.30	0.41
1:A:634:TYR:O	1:A:653:THR:HA	2.20	0.41
1:D:330[B]:ASP:OD2	1:D:599:LYS:HG2	2.20	0.41
1:D:393:PRO:HD2	1:D:415:TYR:CD1	2.55	0.41
1:A:128:HIS:HA	1:A:168:THR:O	2.20	0.41
4:A:804:HDD:HAD2	4:A:804:HDD:HMD3	1.65	0.41
1:B:393:PRO:HD2	1:B:415:TYR:CD1	2.56	0.41
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.55	0.41
1:B:451[B]:MET:HE1	5:D:1570:HOH:O	2.21	0.40
1:B:207:PHE:O	1:B:249:THR:HA	2.21	0.40
1:C:634:TYR:O	1:C:653:THR:HA	2.22	0.40
4:B:804:HDD:HAD2	4:B:804:HDD:HMD3	1.64	0.40
1:D:359:LEU:H	1:D:507:HIS:CD2	2.37	0.40
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.56	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	743/753 (99%)	730 (98%)	12 (2%)	1 (0%)	48	18
1	B	737/753 (98%)	727 (99%)	9 (1%)	1 (0%)	48	18
1	C	737/753 (98%)	726 (98%)	10 (1%)	1 (0%)	48	18
1	D	738/753 (98%)	723 (98%)	14 (2%)	1 (0%)	48	18
All	All	2955/3012 (98%)	2906 (98%)	45 (2%)	4 (0%)	48	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	SER
1	B	75	SER
1	C	75	SER
1	D	75	SER

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	630/636 (99%)	624 (99%)	6 (1%)	68	37
1	B	624/636 (98%)	617 (99%)	7 (1%)	65	33
1	C	624/636 (98%)	618 (99%)	6 (1%)	68	37
1	D	625/636 (98%)	621 (99%)	4 (1%)	78	54
All	All	2503/2544 (98%)	2480 (99%)	23 (1%)	76	42

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	THR
1	A	205	ILE
1	A	377[A]	ARG
1	A	377[B]	ARG
1	A	440[A]	TYR
1	A	440[B]	TYR
1	B	191	THR
1	B	205	ILE
1	B	377[A]	ARG
1	B	377[B]	ARG
1	B	440[A]	TYR
1	B	440[B]	TYR
1	B	565	GLU
1	C	191	THR
1	C	205	ILE
1	C	377[A]	ARG
1	C	377[B]	ARG
1	C	440[A]	TYR
1	C	440[B]	TYR
1	D	191	THR
1	D	205	ILE
1	D	440	TYR
1	D	478	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	507	HIS
1	B	77	ASN
1	B	84	GLN
1	B	507	HIS
1	B	556	GLN
1	B	572	ASN
1	B	682	ASN
1	C	368	GLN
1	C	372	ASN
1	C	507	HIS
1	C	682	ASN
1	D	77	ASN
1	D	139	GLN
1	D	486	GLN

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Mol	Chain	Res	Type
1	D	507	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

15 ligands 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	EDO	A	802	-	3,3,3	0.44	0	2,2,2	0.34	0
3	EDO	B	802	-	3,3,3	0.42	0	2,2,2	0.36	0
4	HDD	A	804	1,5	46,52,52	1.55	9 (19%)	62,89,89	1.47	9 (14%)
4	HDD	C	803	1	46,52,52	1.61	9 (19%)	62,89,89	1.46	10 (16%)
4	HDD	B	804	1,5	46,52,52	1.56	8 (17%)	62,89,89	1.45	11 (17%)
2	GOL	A	801	-	5,5,5	0.85	0	5,5,5	0.80	0
3	EDO	C	802	-	3,3,3	0.47	0	2,2,2	0.33	0
2	GOL	D	1202	-	5,5,5	0.98	0	5,5,5	0.78	0
2	GOL	B	801	-	5,5,5	1.04	0	5,5,5	0.67	0
2	GOL	C	801	-	5,5,5	0.83	0	5,5,5	0.87	0
3	EDO	A	803	-	3,3,3	0.47	0	2,2,2	0.32	0
3	EDO	D	1201	-	3,3,3	0.48	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HDD	D	1204	1,5	46,52,52	1.61	9 (19%)	62,89,89	1.44	8 (12%)
3	EDO	B	803	-	3,3,3	0.46	0	2,2,2	0.36	0
3	EDO	D	1203	-	3,3,3	0.40	0	2,2,2	0.40	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
3	EDO	A	802	-	-	0/1/1/1	-
3	EDO	B	802	-	-	1/1/1/1	-
4	HDD	A	804	1,5	-	4/9/89/89	0/1/9/9
4	HDD	C	803	1	-	4/9/89/89	0/1/9/9
4	HDD	B	804	1,5	-	4/9/89/89	0/1/9/9
2	GOL	A	801	-	-	4/4/4/4	-
3	EDO	C	802	-	-	0/1/1/1	-
2	GOL	D	1202	-	-	0/4/4/4	-
2	GOL	B	801	-	-	2/4/4/4	-
2	GOL	C	801	-	-	0/4/4/4	-
3	EDO	A	803	-	-	0/1/1/1	-
3	EDO	D	1201	-	-	0/1/1/1	-
4	HDD	D	1204	1,5	-	4/9/89/89	0/1/9/9
3	EDO	B	803	-	-	0/1/1/1	-
3	EDO	D	1203	-	-	0/1/1/1	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1204	HDD	CHC-C4B	4.68	1.47	1.38
4	C	803	HDD	CHB-C1B	4.68	1.47	1.38
4	C	803	HDD	CHC-C4B	4.55	1.47	1.38
4	B	804	HDD	CHC-C4B	4.51	1.47	1.38
4	B	804	HDD	CHB-C1B	4.47	1.47	1.38
4	D	1204	HDD	CHB-C1B	4.45	1.47	1.38
4	A	804	HDD	CHC-C4B	4.39	1.47	1.38
4	A	804	HDD	CHB-C1B	4.32	1.46	1.38
4	B	804	HDD	C4B-NB	-2.92	1.34	1.39
4	D	1204	HDD	C4B-NB	-2.91	1.34	1.39
4	D	1204	HDD	C4C-NC	-2.90	1.34	1.39
4	A	804	HDD	C4B-NB	-2.84	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	803	HDD	C4A-NA	-2.78	1.34	1.39
4	C	803	HDD	C4C-NC	-2.78	1.34	1.39
4	A	804	HDD	C4C-NC	-2.76	1.34	1.39
4	B	804	HDD	C4A-NA	-2.71	1.34	1.39
4	A	804	HDD	C4A-NA	-2.69	1.34	1.39
4	B	804	HDD	C1B-NB	-2.65	1.34	1.39
4	D	1204	HDD	C4A-NA	-2.65	1.34	1.39
4	D	1204	HDD	C1B-NB	-2.63	1.34	1.39
4	C	803	HDD	C1C-NC	-2.58	1.34	1.39
4	C	803	HDD	C4B-NB	-2.55	1.34	1.39
4	D	1204	HDD	C1A-NA	-2.54	1.34	1.39
4	B	804	HDD	C1A-NA	-2.50	1.34	1.39
4	B	804	HDD	C1C-NC	-2.48	1.34	1.39
4	D	1204	HDD	C1C-NC	-2.45	1.35	1.39
4	C	803	HDD	C1B-NB	-2.44	1.35	1.39
4	C	803	HDD	C1A-NA	-2.40	1.35	1.39
4	B	804	HDD	C4C-NC	-2.38	1.35	1.39
4	A	804	HDD	C1C-NC	-2.36	1.35	1.39
4	A	804	HDD	C1B-NB	-2.35	1.35	1.39
4	A	804	HDD	C1A-NA	-2.27	1.35	1.39
4	D	1204	HDD	C1B-C2B	-2.18	1.41	1.45
4	A	804	HDD	C1C-C2C	2.09	1.48	1.43
4	C	803	HDD	C1C-C2C	2.08	1.48	1.43

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1204	HDD	O1D-CGD-O2D	4.12	124.28	120.81
4	C	803	HDD	C3C-C2C-C1C	-4.06	102.38	107.17
4	C	803	HDD	C3B-C2B-C1B	-4.01	103.25	107.05
4	A	804	HDD	C3B-C2B-C1B	-3.97	103.29	107.05
4	C	803	HDD	O1D-CGD-O2D	3.97	124.15	120.81
4	D	1204	HDD	C3B-C2B-C1B	-3.94	103.31	107.05
4	B	804	HDD	O1D-CGD-O2D	3.91	124.11	120.81
4	A	804	HDD	O1D-CGD-O2D	3.79	124.01	120.81
4	D	1204	HDD	C3C-C2C-C1C	-3.71	102.80	107.17
4	A	804	HDD	C3C-C2C-C1C	-3.55	102.98	107.17
4	B	804	HDD	C3B-C2B-C1B	-3.50	103.74	107.05
4	B	804	HDD	C2D-C1D-CHD	-3.34	119.08	124.27
4	C	803	HDD	C2B-C1B-NB	3.33	115.80	109.64
4	A	804	HDD	C2B-C1B-NB	3.29	115.73	109.64
4	B	804	HDD	C3C-C2C-C1C	-3.28	103.30	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1204	HDD	C2D-C1D-CHD	-3.15	119.38	124.27
4	D	1204	HDD	C2B-C1B-NB	3.13	115.43	109.64
4	A	804	HDD	C2D-C1D-CHD	-2.99	119.62	124.27
4	B	804	HDD	C2B-C1B-NB	2.80	114.82	109.64
4	C	803	HDD	C2D-C1D-CHD	-2.79	119.94	124.27
4	C	803	HDD	CBD-CAD-C3D	2.53	107.58	103.98
4	B	804	HDD	CBD-CAD-C3D	2.50	107.54	103.98
4	A	804	HDD	CHB-C1B-NB	-2.47	121.76	124.45
4	B	804	HDD	O1D-CGD-CBD	2.47	112.42	110.17
4	B	804	HDD	CHB-C1B-NB	-2.43	121.81	124.45
4	A	804	HDD	CBD-CAD-C3D	2.37	107.35	103.98
4	A	804	HDD	O1D-CGD-CBD	2.33	112.30	110.17
4	C	803	HDD	CHB-C1B-NB	-2.30	121.94	124.45
4	B	804	HDD	C2C-C1C-NC	2.29	113.82	110.14
4	A	804	HDD	C3C-C4C-NC	2.28	111.72	109.80
4	C	803	HDD	O1D-CGD-CBD	2.23	112.21	110.17
4	D	1204	HDD	C2C-C1C-NC	2.15	113.59	110.14
4	D	1204	HDD	CAA-CBA-CGA	-2.13	108.01	113.67
4	D	1204	HDD	CBD-CAD-C3D	2.13	107.02	103.98
4	C	803	HDD	C2C-C1C-NC	2.13	113.55	110.14
4	B	804	HDD	C3C-C4C-NC	2.02	111.50	109.80
4	B	804	HDD	CMC-C2C-C3C	2.00	131.27	126.55
4	C	803	HDD	CAA-CBA-CGA	-2.00	108.35	113.67

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	GOL	O1-C1-C2-C3
2	B	801	GOL	O1-C1-C2-C3
2	A	801	GOL	C1-C2-C3-O3
2	A	801	GOL	O1-C1-C2-O2
2	B	801	GOL	O1-C1-C2-O2
4	B	804	HDD	C2B-C3B-CAB-CBB
4	C	803	HDD	C2B-C3B-CAB-CBB
3	B	802	EDO	O1-C1-C2-O2
4	A	804	HDD	CAA-CBA-CGA-O2A
4	C	803	HDD	CAA-CBA-CGA-O2A
4	D	1204	HDD	CAA-CBA-CGA-O2A
4	B	804	HDD	CAA-CBA-CGA-O1A
4	B	804	HDD	CAA-CBA-CGA-O2A
4	A	804	HDD	CAA-CBA-CGA-O1A

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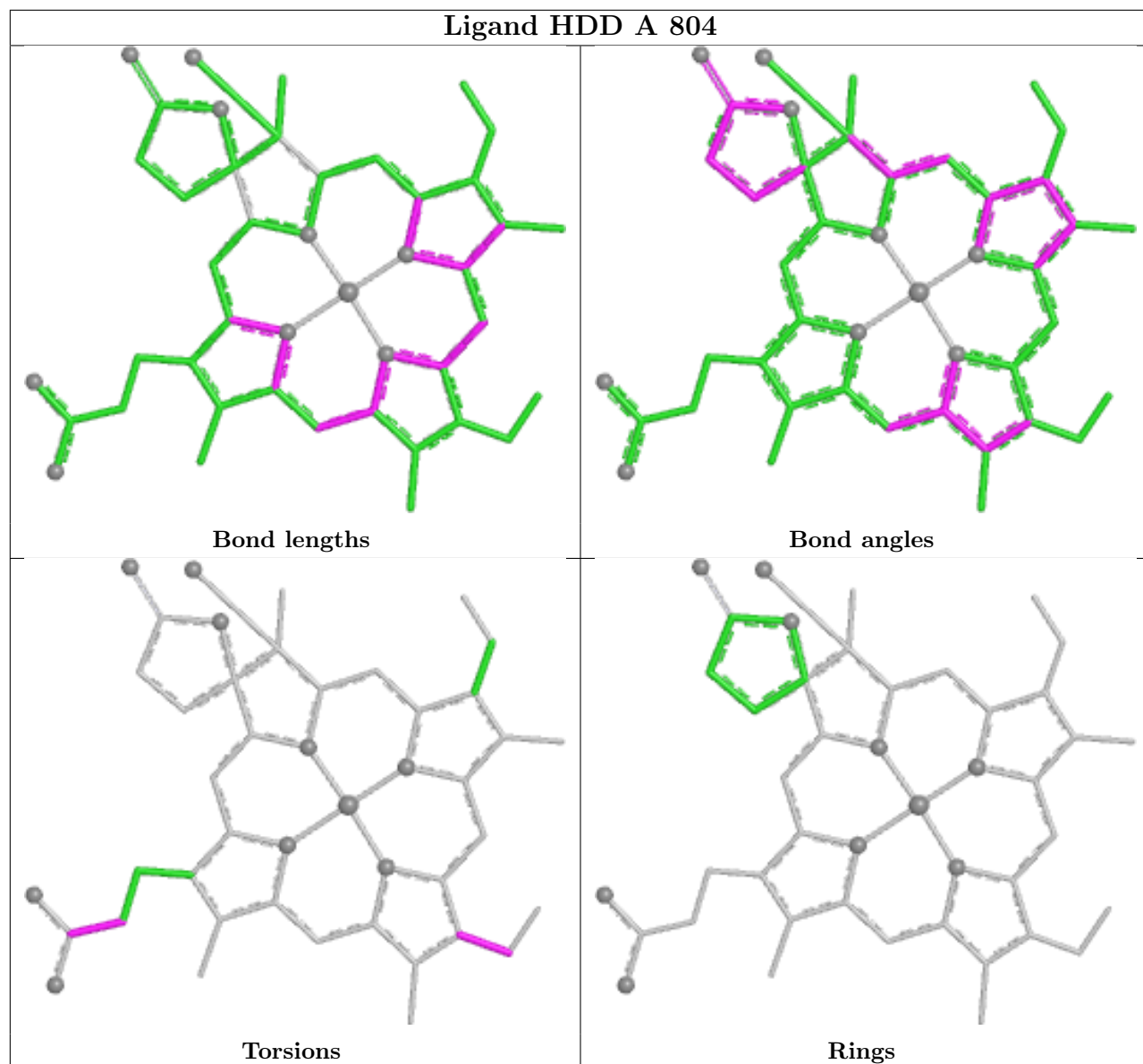
Mol	Chain	Res	Type	Atoms
4	C	803	HDD	CAA-CBA-CGA-O1A
4	D	1204	HDD	CAA-CBA-CGA-O1A
4	A	804	HDD	C2B-C3B-CAB-CBB
4	A	804	HDD	C4B-C3B-CAB-CBB
4	B	804	HDD	C4B-C3B-CAB-CBB
4	C	803	HDD	C4B-C3B-CAB-CBB
4	D	1204	HDD	C4B-C3B-CAB-CBB
2	A	801	GOL	O2-C2-C3-O3
4	D	1204	HDD	C2B-C3B-CAB-CBB

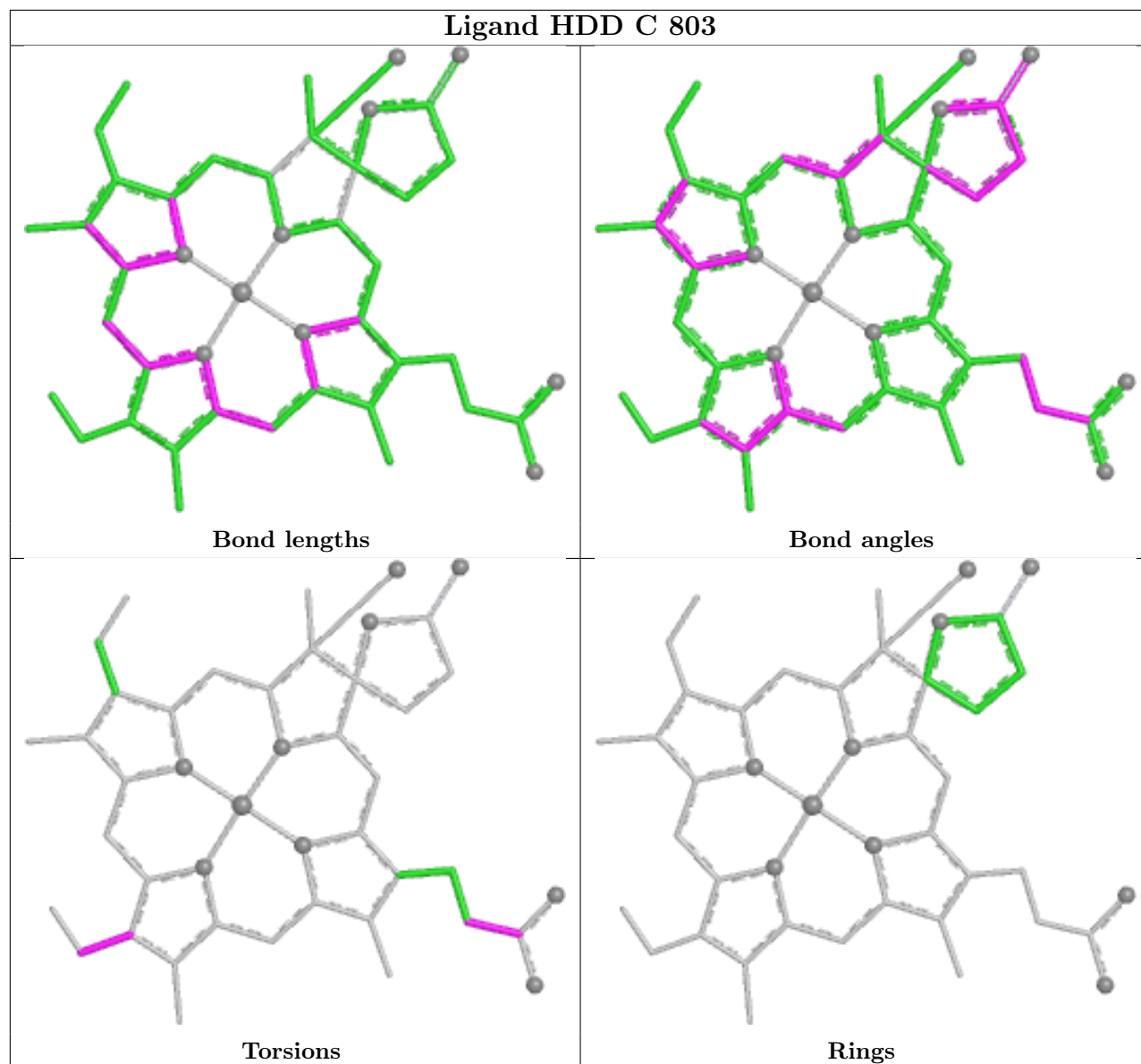
There are no ring outliers.

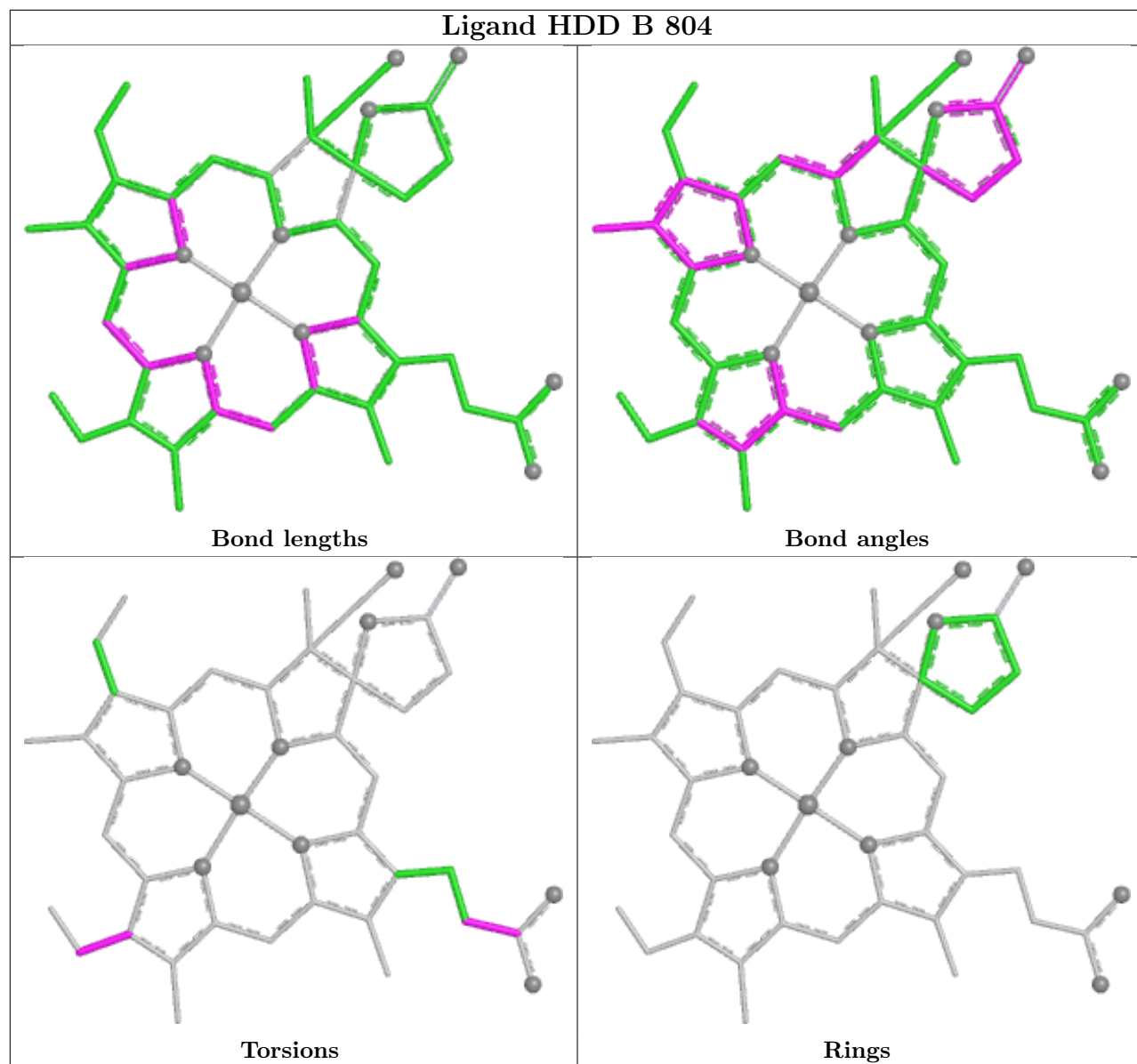
10 monomers are involved in 16 short contacts:

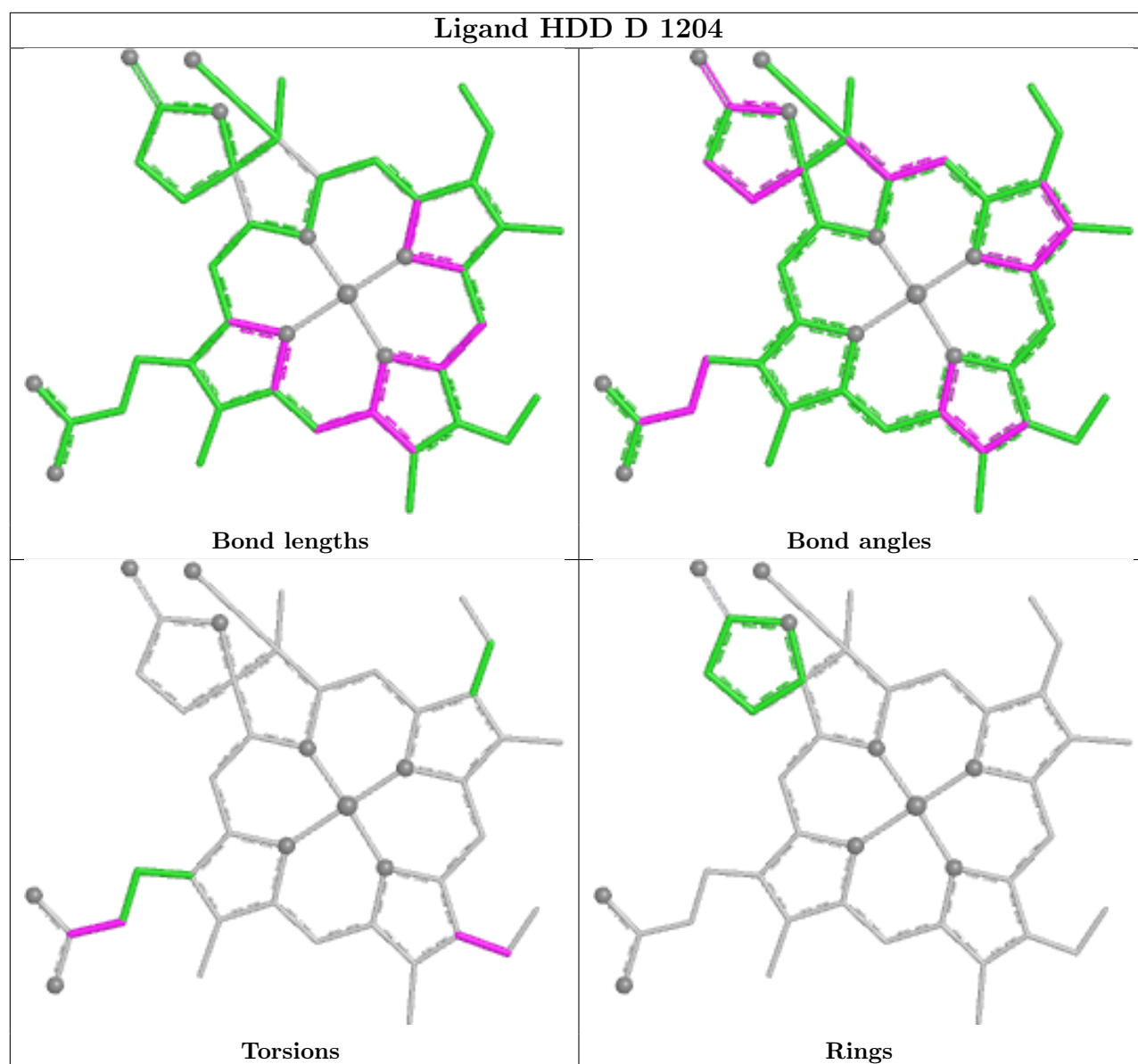
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	EDO	3	0
4	A	804	HDD	2	0
4	C	803	HDD	2	0
4	B	804	HDD	2	0
3	C	802	EDO	1	0
3	A	803	EDO	1	0
3	D	1201	EDO	1	0
4	D	1204	HDD	2	0
3	B	803	EDO	1	0
3	D	1203	EDO	1	0

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	727/753 (96%)	-0.45	7 (0%) 79 82	4, 12, 24, 47	18 (2%)
1	B	727/753 (96%)	-0.29	6 (0%) 82 86	6, 14, 31, 50	12 (1%)
1	C	727/753 (96%)	-0.31	8 (1%) 78 81	5, 14, 31, 49	12 (1%)
1	D	727/753 (96%)	-0.44	3 (0%) 88 91	5, 12, 25, 45	13 (1%)
All	All	2908/3012 (96%)	-0.37	24 (0%) 82 86	4, 13, 29, 50	55 (1%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	749	ASP	3.8
1	A	751	ILE	3.7
1	B	726	GLY	3.3
1	C	724	ALA	3.0
1	B	725	ASP	3.0
1	D	712	ASP	3.0
1	C	726	GLY	2.9
1	D	710	ILE	2.8
1	A	596	GLY	2.6
1	C	596	GLY	2.6
1	D	596	GLY	2.5
1	B	27	ASP	2.5
1	A	27	ASP	2.4
1	C	27	ASP	2.4
1	C	725	ASP	2.4
1	B	596	GLY	2.3
1	C	641	THR	2.2
1	C	595	ASP	2.1
1	A	748[A]	ILE	2.1
1	B	713	GLN	2.1
1	C	727	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	595	ASP	2.0
1	A	597	ASP	2.0
1	B	597	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

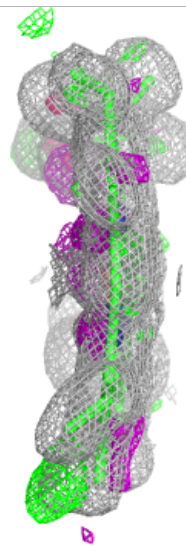
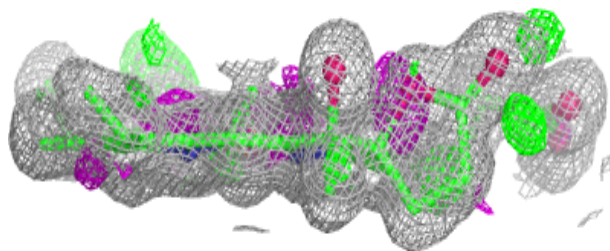
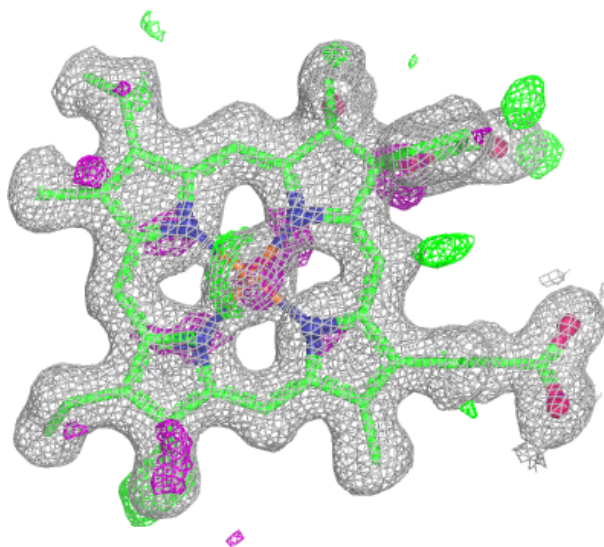
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	B	802	4/4	0.78	0.18	34,35,35,36	0
3	EDO	D	1203	4/4	0.83	0.17	44,45,46,47	0
3	EDO	D	1201	4/4	0.84	0.15	33,34,34,35	0
3	EDO	A	802	4/4	0.84	0.17	51,52,52,52	0
3	EDO	A	803	4/4	0.86	0.14	29,30,30,31	0
2	GOL	A	801	6/6	0.86	0.13	20,21,23,24	0
3	EDO	C	802	4/4	0.87	0.13	31,31,31,32	0
3	EDO	B	803	4/4	0.88	0.13	32,34,35,35	0
2	GOL	B	801	6/6	0.92	0.11	19,23,25,25	0
2	GOL	D	1202	6/6	0.93	0.09	16,20,21,21	0
2	GOL	C	801	6/6	0.97	0.07	17,19,20,21	0
4	HDD	B	804	44/44	0.98	0.06	9,11,17,18	0
4	HDD	A	804	44/44	0.99	0.06	8,10,16,17	0
4	HDD	C	803	44/44	0.99	0.06	9,11,16,17	0
4	HDD	D	1204	44/44	0.99	0.06	8,10,15,18	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.

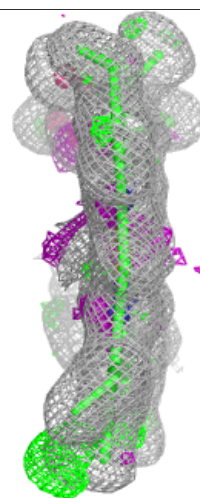
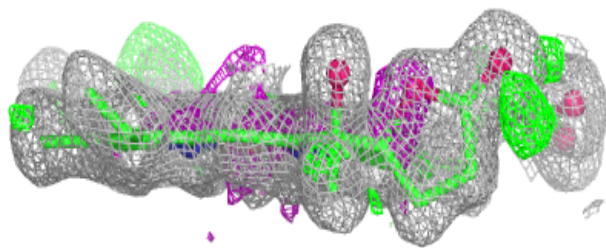
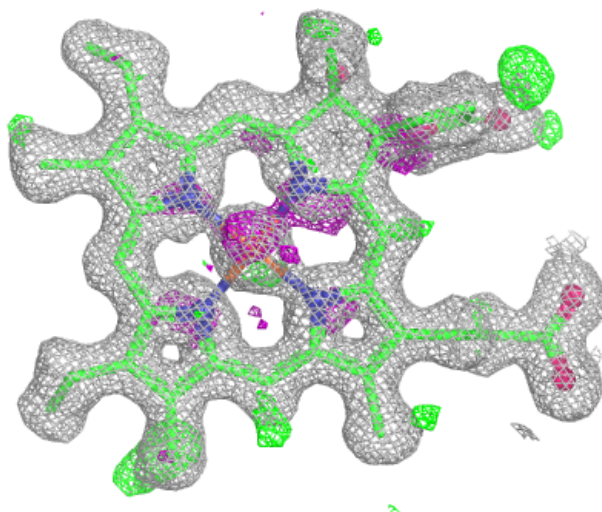
Electron density around HDD B 804:

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



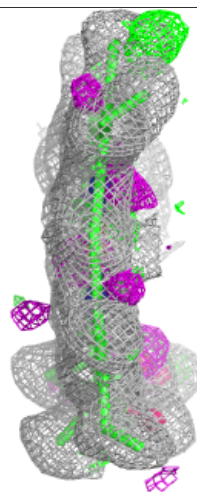
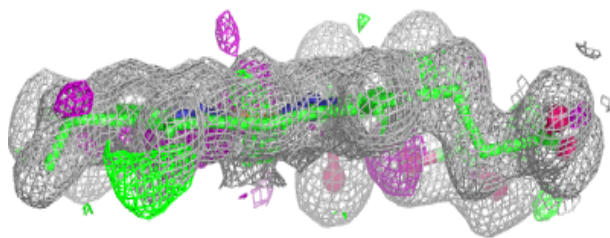
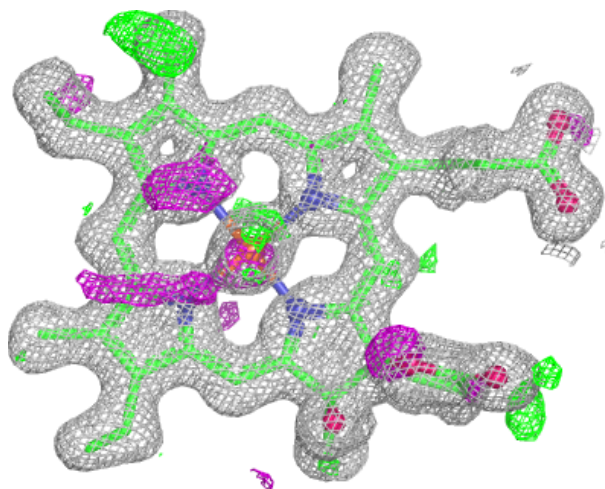
Electron density around HDD A 804:

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



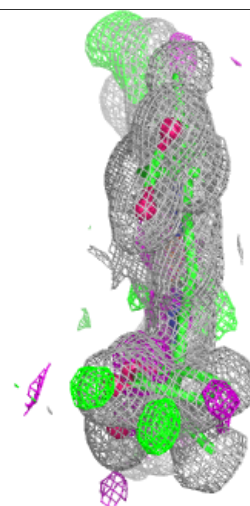
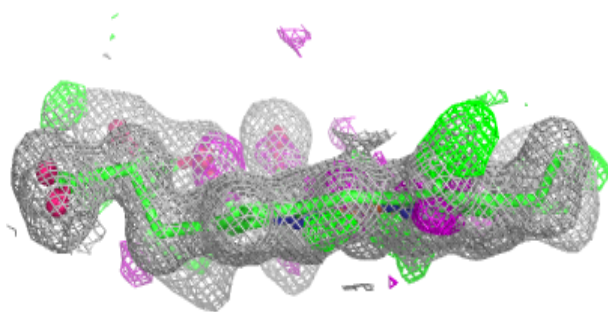
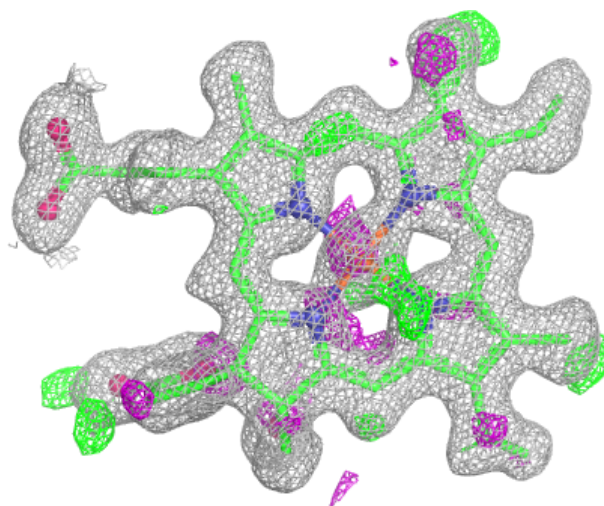
Electron density around HDD C 803:

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



Electron density around HDD D 1204:

$2mF_o-DF_c$ (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.