



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 24, 2021 – 11:51 AM GMT

PDB ID : 6ZTX
Title : Crystal Structure of catalase HPII 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 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 : 2.17.1.dev1
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) : 2.17.1.dev1

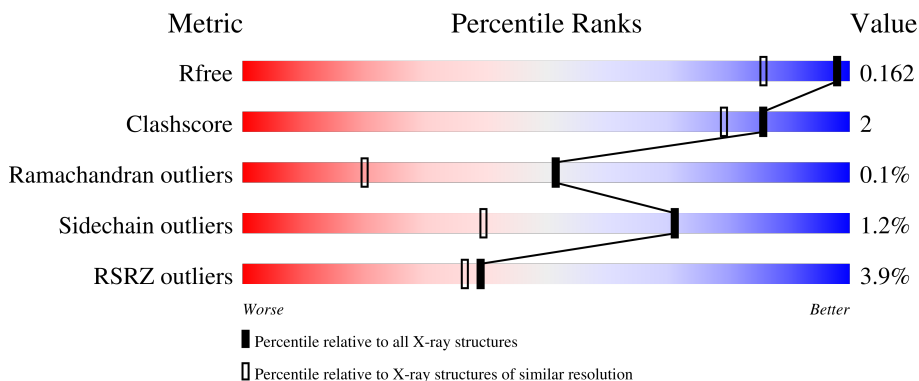
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

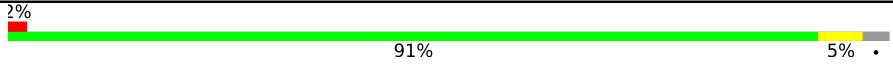
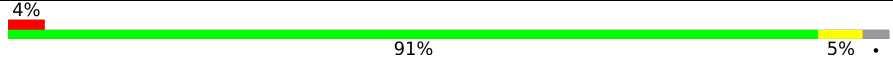
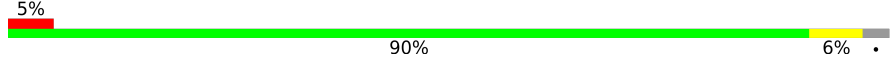
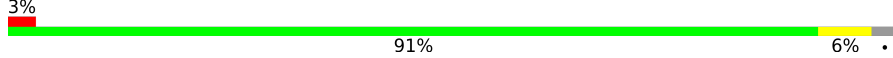
The reported resolution of this entry is 1.30 Å.

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}	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (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	 2% 91% 5%
1	B	753	 4% 91% 5%
1	C	753	 5% 90% 6%
1	D	753	 3% 91% 6%

2 Entry composition [i](#)

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 HP11.

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

There are 16 discrepancies between the modelled and reference sequences:

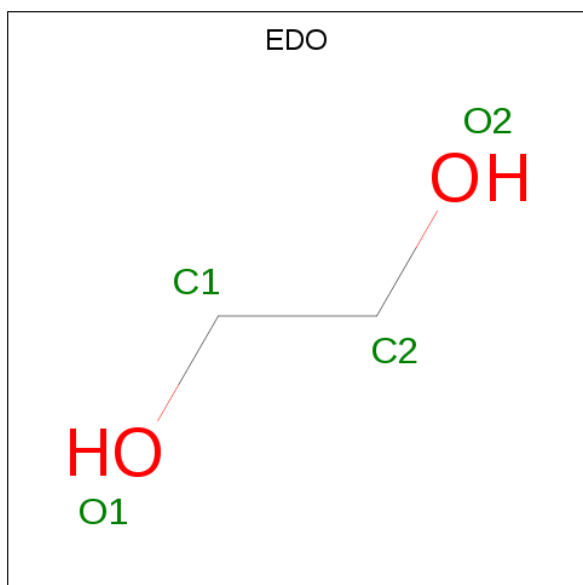
Chain	Residue	Modelled	Actual	Comment	Reference
A	37	SER	ARG	variant	UNP P21179
A	99	ASP	SER	variant	UNP P21179
A	372	ASN	LYS	variant	UNP P21179
A	521	SER	ARG	variant	UNP P21179
B	37	SER	ARG	variant	UNP P21179
B	99	ASP	SER	variant	UNP P21179
B	372	ASN	LYS	variant	UNP P21179
B	521	SER	ARG	variant	UNP 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 (three-letter code: GOL) (formula: C₃H₈O₃).



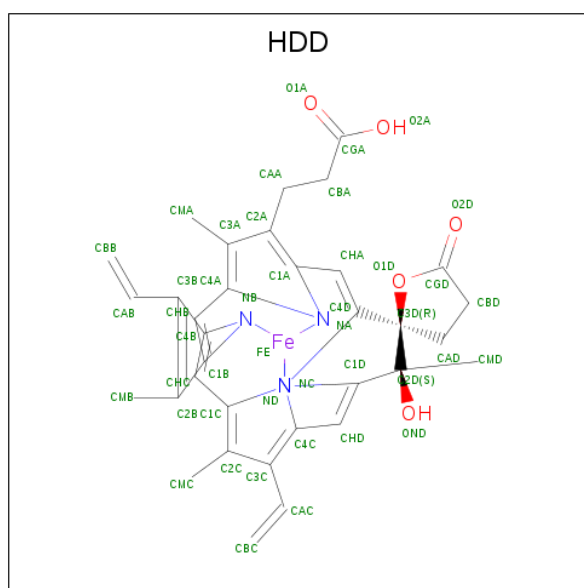
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (three-letter code: 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 44 34 1 4 5	0	0
4	B	1	Total C Fe N O 44 34 1 4 5	0	0
4	C	1	Total C Fe N O 44 34 1 4 5	0	0
4	D	1	Total C Fe N O 44 34 1 4 5	0	0

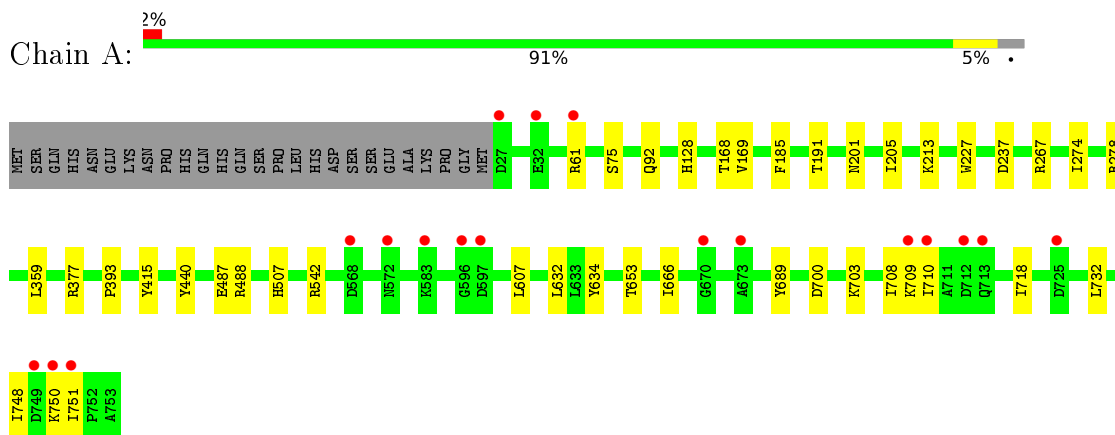
- Molecule 5 is water.

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

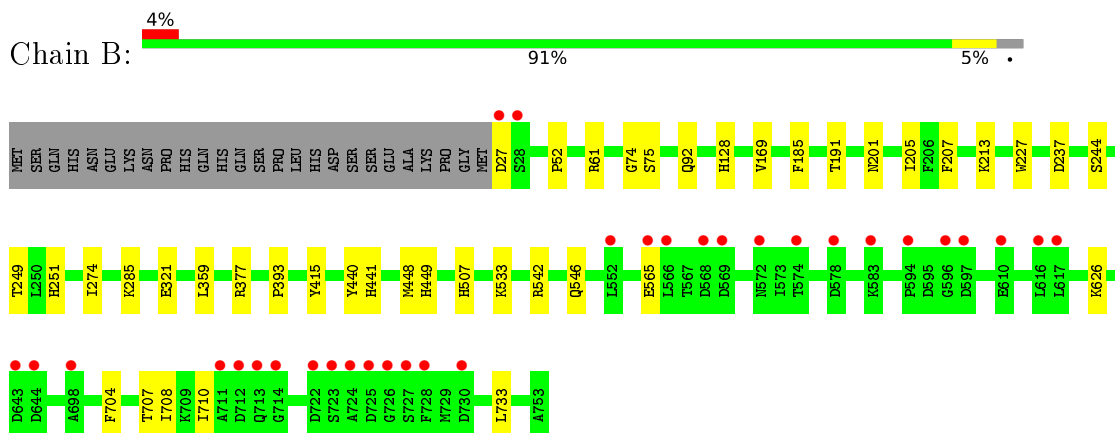
3 Residue-property plots [i](#)

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.

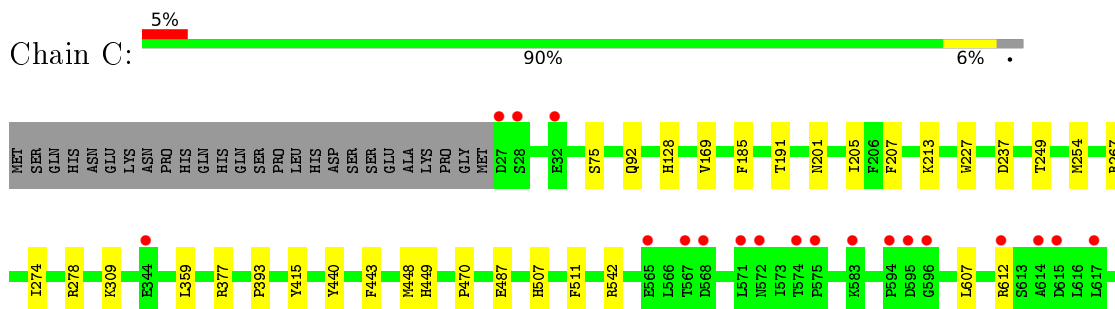
- Molecule 1: Catalase HPII

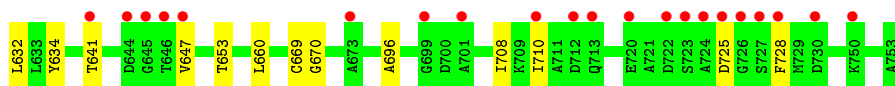


- Molecule 1: Catalase HPII

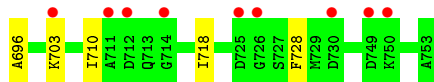
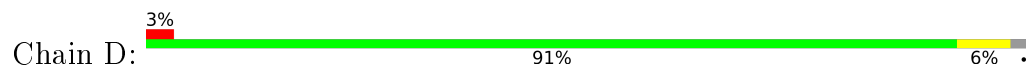


- Molecule 1: Catalase HPII





- Molecule 1: Catalase HP11



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)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.135 , 0.162 0.135 , 0.162	Depositor DCC
R_{free} test set	1331 reflections (0.20%)	wwPDB-VP
Wilson B-factor (Å ²)	11.4	Xtrriage
Anisotropy	0.216	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtrriage
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

Xtrriage'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: HDD, GOL, EDO

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	0.32	0/6048	0.55	0/8220
1	B	0.31	0/5999	0.54	0/8156
1	C	0.30	0/5996	0.53	0/8152
1	D	0.32	0/6001	0.55	0/8157
All	All	0.31	0/24044	0.54	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	24	0
1	B	5826	0	5642	25	0
1	C	5826	0	5637	24	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	4	0
4	C	44	0	31	2	0
4	D	44	0	31	3	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	8	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:274:ILE:HD12	4:B:804:HDD:HMB1	1.90	0.53
1:C:201:ASN:CG	4:C:803:HDD:HMB2	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:LEU:H	1:B:507:HIS:HD2	1.57	0.53
1:C:254[B]:MET:HG2	1:C:511:PHE:HD2	1.72	0.53
1:D:201:ASN:CG	4:D:1204:HDD:HMB2	2.28	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:201:ASN:CG	4:B:804:HDD:HMB2	2.30	0.51
1:B:533:LYS:NZ	5:B:908:HOH:O	2.40	0.51
1:C:274:ILE:HD12	4:C:803:HDD:HMB1	1.93	0.51
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: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:201:ASN:CG	4:A:804:HDD:HMB2	2.33	0.49
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:274:ILE:HD12	4:D:1204:HDD:HMB1	1.95	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: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: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:A:274:ILE:HD12	4:A:804:HDD:HMB1	1.97	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: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
1:B:285:LYS:NZ	5:B:910:HOH:O	2.42	0.45
1:D:607:LEU:HD22	1:D:611:VAL:HG21	1.97	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:LYS:HD2	1:C:660:LEU:HD11	1.99	0.43
1:A:278:ARG:HH22	1:A:487[B]:GLU:CD	2.22	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:C:278:ARG:HH22	1:C:487[B]:GLU:CD	2.21	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:278:ARG:HH22	1:D:487[B]:GLU:CD	2.23	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:B:201:ASN:ND2	4:B:804:HDD:HMB2	2.35	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:B:804:HDD:HMD2	4:B:804:HDD:HAD2	1.86	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: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
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 [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	743/753 (99%)	730 (98%)	12 (2%)	1 (0%)	51	20
1	B	737/753 (98%)	727 (99%)	9 (1%)	1 (0%)	51	20
1	C	737/753 (98%)	726 (98%)	10 (1%)	1 (0%)	51	20
1	D	738/753 (98%)	723 (98%)	14 (2%)	1 (0%)	51	20
All	All	2955/3012 (98%)	2906 (98%)	45 (2%)	4 (0%)	51	20

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	630/636 (99%)	621 (99%)	9 (1%)	67	34
1	B	624/636 (98%)	613 (98%)	11 (2%)	59	24
1	C	624/636 (98%)	615 (99%)	9 (1%)	67	34
1	D	625/636 (98%)	619 (99%)	6 (1%)	76	48
All	All	2503/2544 (98%)	2468 (99%)	35 (1%)	71	34

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	PHE
1	A	191	THR
1	A	205	ILE
1	A	227	TRP
1	A	237	ASP
1	A	377[A]	ARG
1	A	377[B]	ARG
1	A	440[A]	TYR
1	A	440[B]	TYR
1	B	61	ARG
1	B	185	PHE
1	B	191	THR
1	B	205	ILE
1	B	227	TRP
1	B	237	ASP
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	185	PHE
1	C	191	THR
1	C	205	ILE
1	C	227	TRP
1	C	237	ASP
1	C	377[A]	ARG
1	C	377[B]	ARG
1	C	440[A]	TYR
1	C	440[B]	TYR
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	227	TRP
1	D	237	ASP
1	D	440	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	507	HIS
1	B	507	HIS

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Mol	Chain	Res	Type
1	C	507	HIS
1	D	507	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	D	1203	-	3,3,3	0.43	0	2,2,2	0.35	0
4	HDD	B	804	1,5	38,52,52	0.70	0	28,89,89	1.74	6 (21%)
4	HDD	C	803	1	38,52,52	0.74	0	28,89,89	1.57	6 (21%)
3	EDO	A	802	-	3,3,3	0.47	0	2,2,2	0.30	0
2	GOL	B	801	-	5,5,5	1.01	0	5,5,5	0.62	0
3	EDO	D	1201	-	3,3,3	0.51	0	2,2,2	0.23	0
2	GOL	D	1202	-	5,5,5	0.95	0	5,5,5	0.72	0
4	HDD	D	1204	1,5	38,52,52	0.74	1 (2%)	28,89,89	1.68	6 (21%)
3	EDO	C	802	-	3,3,3	0.50	0	2,2,2	0.29	0
3	EDO	A	803	-	3,3,3	0.51	0	2,2,2	0.27	0
3	EDO	B	802	-	3,3,3	0.45	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	801	-	5,5,5	0.82	0	5,5,5	0.74	0
3	EDO	B	803	-	3,3,3	0.49	0	2,2,2	0.32	0
4	HDD	A	804	1,5	38,52,52	0.67	0	28,89,89	1.66	7 (25%)
2	GOL	C	801	-	5,5,5	0.80	0	5,5,5	0.80	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	D	1203	-	-	0/1/1/1	-
4	HDD	B	804	1,5	-	0/3/89/89	0/1/9/9
4	HDD	C	803	1	-	0/3/89/89	0/1/9/9
3	EDO	A	802	-	-	0/1/1/1	-
2	GOL	B	801	-	-	2/4/4/4	-
3	EDO	D	1201	-	-	0/1/1/1	-
2	GOL	D	1202	-	-	0/4/4/4	-
4	HDD	D	1204	1,5	-	0/3/89/89	0/1/9/9
3	EDO	C	802	-	-	0/1/1/1	-
3	EDO	A	803	-	-	0/1/1/1	-
3	EDO	B	802	-	-	1/1/1/1	-
2	GOL	A	801	-	-	3/4/4/4	-
3	EDO	B	803	-	-	0/1/1/1	-
4	HDD	A	804	1,5	-	0/3/89/89	0/1/9/9
2	GOL	C	801	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1204	HDD	CAA-C2A	-2.07	1.49	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1204	HDD	O1D-CGD-O2D	3.90	124.28	120.80
4	C	803	HDD	O1D-CGD-O2D	3.76	124.15	120.80
4	B	804	HDD	O1D-CGD-O2D	3.71	124.11	120.80
4	A	804	HDD	O1D-CGD-O2D	3.59	124.01	120.80
4	B	804	HDD	CMC-C2C-C3C	3.52	131.27	124.68
4	A	804	HDD	CMC-C2C-C3C	3.32	130.88	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	804	HDD	C2D-C1D-CHD	-3.15	119.08	124.28
4	C	803	HDD	CMC-C2C-C3C	3.10	130.48	124.68
4	D	1204	HDD	CMC-C2C-C3C	3.05	130.38	124.68
4	D	1204	HDD	C2D-C1D-CHD	-2.97	119.38	124.28
4	A	804	HDD	C2D-C1D-CHD	-2.82	119.62	124.28
4	D	1204	HDD	CAA-CBA-CGA	-2.78	108.01	112.67
4	D	1204	HDD	CMB-C2B-C3B	2.71	129.75	124.68
4	C	803	HDD	C2D-C1D-CHD	-2.63	119.94	124.28
4	A	804	HDD	CMB-C2B-C3B	2.60	129.54	124.68
4	C	803	HDD	CAA-CBA-CGA	-2.58	108.35	112.67
4	B	804	HDD	CAA-CBA-CGA	-2.54	108.41	112.67
4	C	803	HDD	CMB-C2B-C3B	2.47	129.30	124.68
4	A	804	HDD	CAA-CBA-CGA	-2.44	108.58	112.67
4	B	804	HDD	O1D-CGD-CBD	2.22	112.42	110.19
4	A	804	HDD	O1D-CGD-CBD	2.09	112.30	110.19
4	D	1204	HDD	CMA-C3A-C4A	-2.09	125.25	128.46
4	B	804	HDD	CMA-C3A-C4A	-2.08	125.27	128.46
4	A	804	HDD	CMA-C3A-C4A	-2.05	125.32	128.46
4	C	803	HDD	O1D-CGD-CBD	2.00	112.21	110.19

There are no chirality outliers.

All (6) 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
3	B	802	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 19 short contacts:

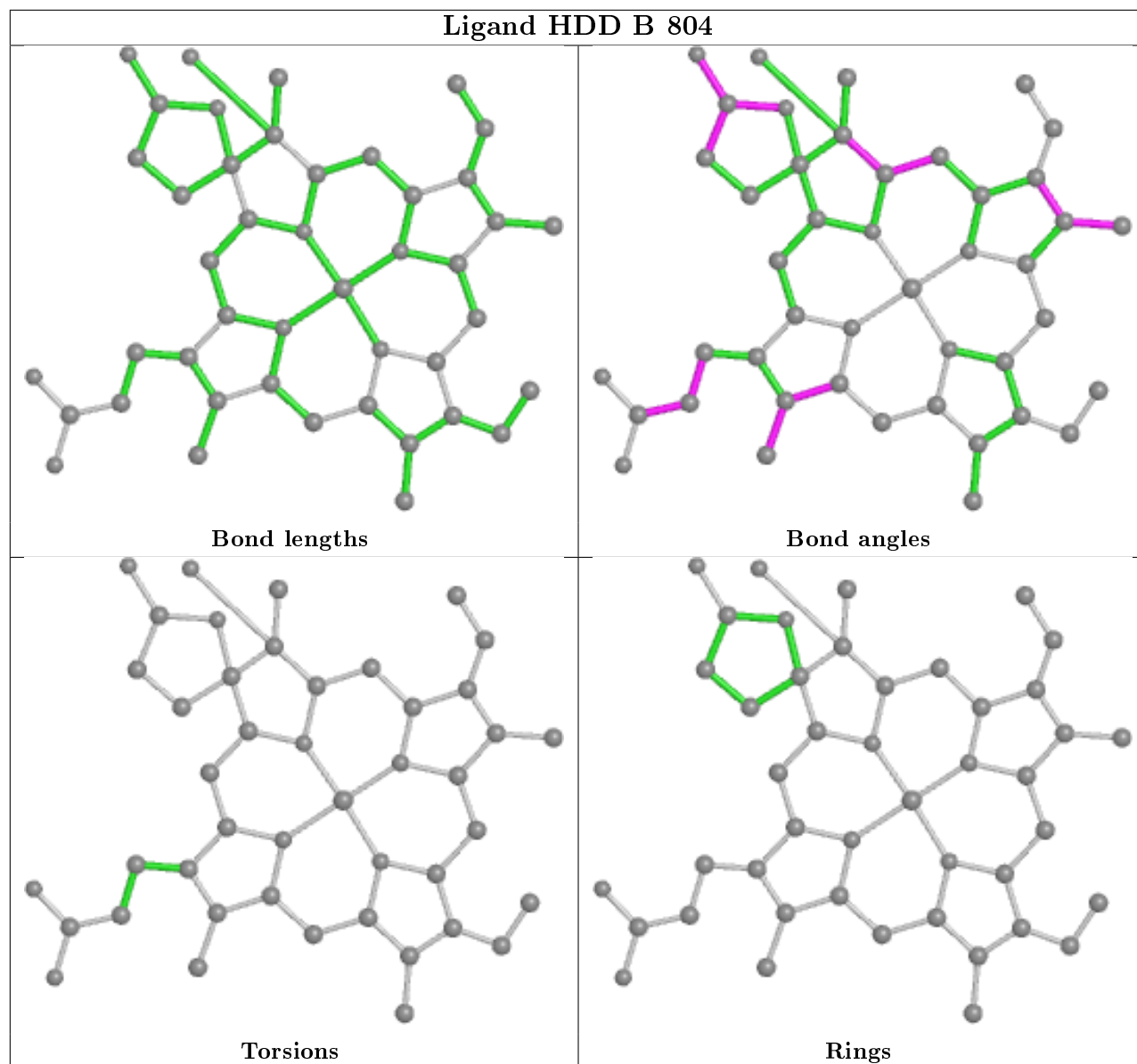
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1203	EDO	1	0
4	B	804	HDD	4	0
4	C	803	HDD	2	0
3	D	1201	EDO	1	0
4	D	1204	HDD	3	0
3	C	802	EDO	1	0

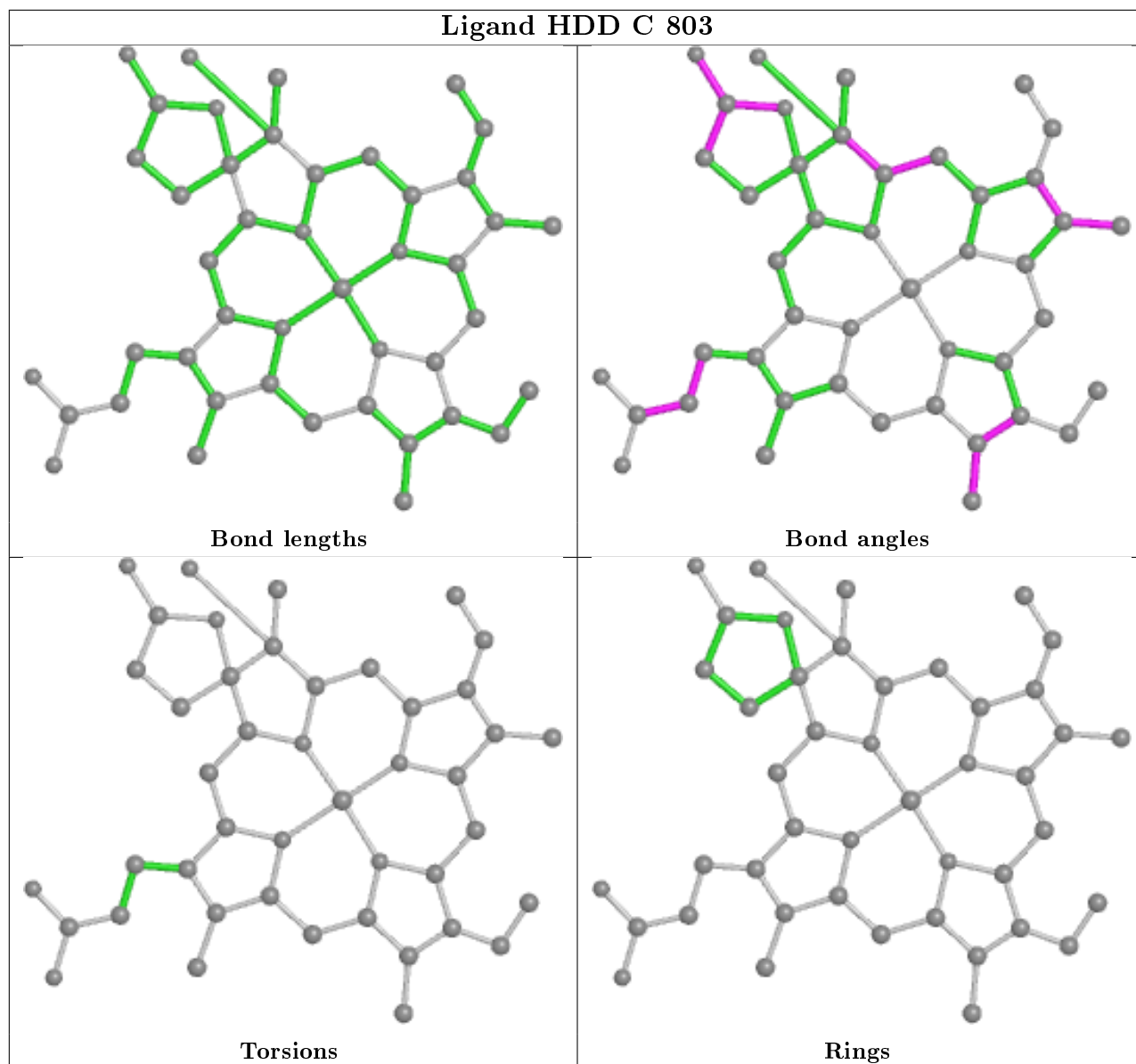
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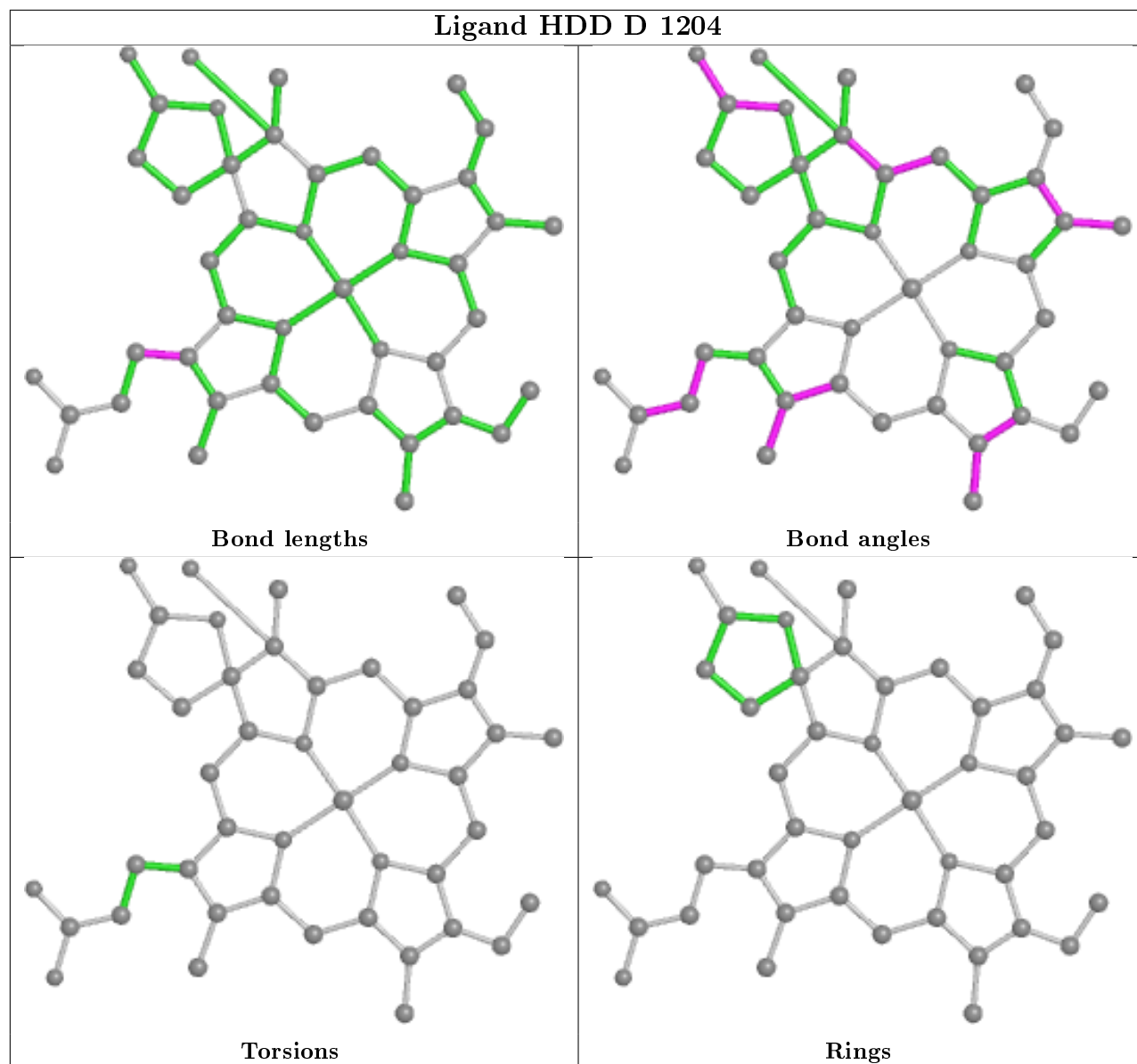
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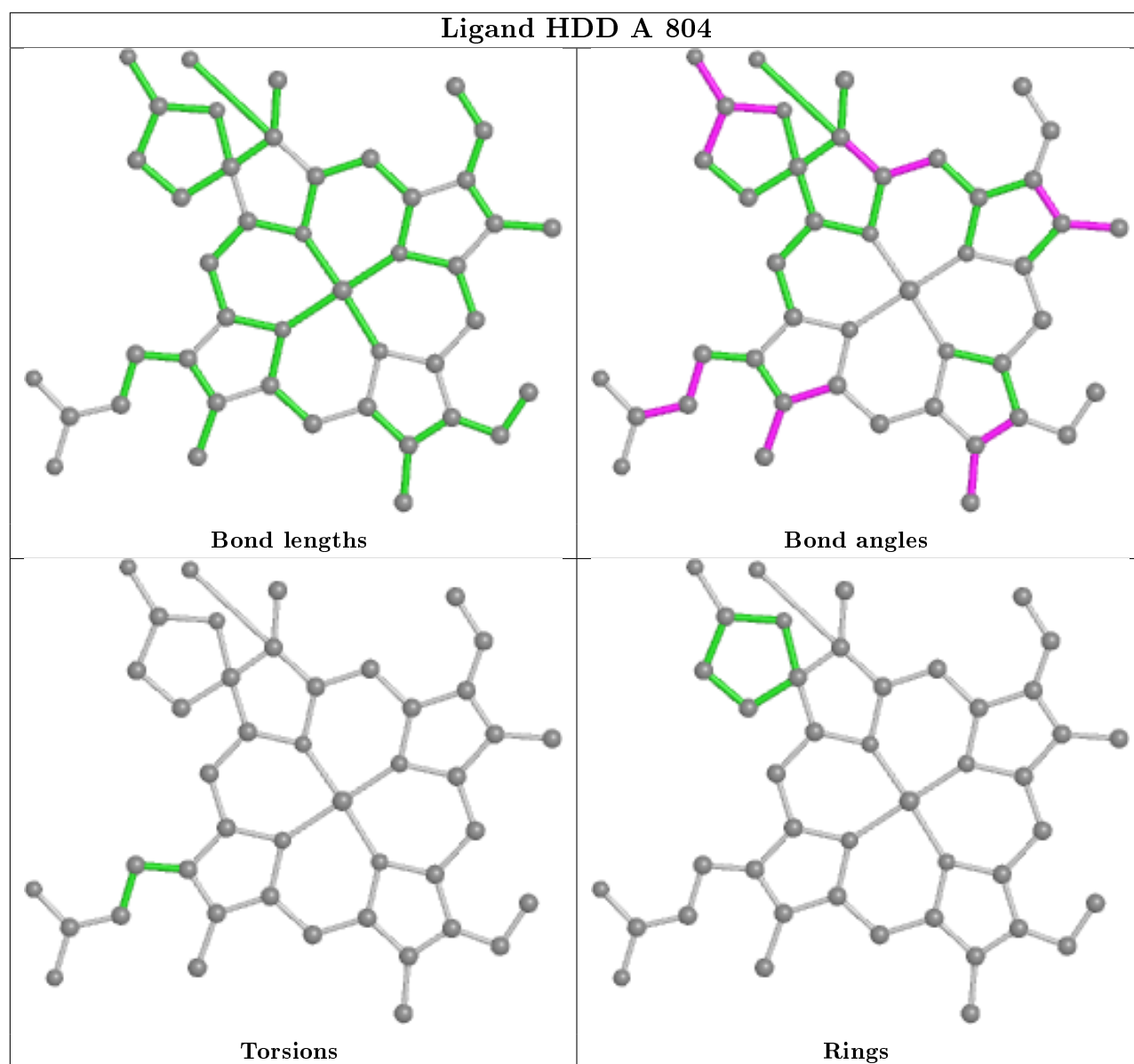
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	EDO	1	0
3	B	802	EDO	3	0
3	B	803	EDO	1	0
4	A	804	HDD	2	0

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%)	0.06	18 (2%) 57 56	8, 12, 24, 47	0
1	B	727/753 (96%)	0.17	32 (4%) 34 32	8, 14, 31, 50	0
1	C	727/753 (96%)	0.21	40 (5%) 25 22	8, 14, 31, 49	0
1	D	727/753 (96%)	0.07	22 (3%) 50 48	8, 12, 25, 45	0
All	All	2908/3012 (96%)	0.13	112 (3%) 39 36	8, 13, 29, 50	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	726	GLY	6.3
1	B	726	GLY	6.0
1	D	596	GLY	5.7
1	B	725	ASP	5.2
1	C	27	ASP	5.2
1	A	751	ILE	4.9
1	B	568	ASP	4.8
1	B	27	ASP	4.6
1	C	647	VAL	4.6
1	C	28	SER	4.4
1	D	726	GLY	4.4
1	C	724	ALA	4.3
1	A	596	GLY	4.2
1	A	749	ASP	4.2
1	A	750	LYS	4.1
1	D	712	ASP	4.1
1	D	583	LYS	4.0
1	B	617	LEU	4.0
1	C	32	GLU	3.9
1	A	597	ASP	3.8
1	D	597	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	583	LYS	3.7
1	D	32	GLU	3.7
1	D	617	LEU	3.7
1	C	596	GLY	3.6
1	B	565	GLU	3.6
1	C	712	ASP	3.5
1	B	552	LEU	3.5
1	B	594	PRO	3.5
1	C	568	ASP	3.5
1	C	612	ARG	3.4
1	D	27	ASP	3.4
1	B	596	GLY	3.4
1	A	27	ASP	3.4
1	B	572	ASN	3.3
1	B	583	LYS	3.3
1	C	572	ASN	3.3
1	C	646	THR	3.2
1	C	722	ASP	3.2
1	C	725	ASP	3.2
1	D	28	SER	3.2
1	B	712	ASP	3.2
1	C	617	LEU	3.1
1	B	713	GLN	3.1
1	B	727	SER	3.1
1	A	568	ASP	3.0
1	C	723	SER	2.9
1	C	574	THR	2.9
1	C	728	PHE	2.9
1	A	583	LYS	2.9
1	C	750	LYS	2.8
1	B	724	ALA	2.8
1	B	711	ALA	2.7
1	A	712	ASP	2.7
1	B	597	ASP	2.7
1	D	750	LYS	2.6
1	B	28	SER	2.6
1	C	673	ALA	2.6
1	A	673	ALA	2.6
1	C	713	GLN	2.6
1	C	641	THR	2.6
1	D	711	ALA	2.5
1	C	571	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	710	ILE	2.5
1	C	344	GLU	2.5
1	B	722	ASP	2.5
1	A	709	LYS	2.5
1	D	568	ASP	2.4
1	C	567	THR	2.4
1	C	595	ASP	2.4
1	A	725	ASP	2.4
1	D	574	THR	2.4
1	C	614	ALA	2.3
1	B	569	ASP	2.3
1	D	725	ASP	2.3
1	C	565	GLU	2.3
1	D	572	ASN	2.2
1	C	699	GLY	2.2
1	D	730	ASP	2.2
1	C	727	SER	2.2
1	B	730	ASP	2.2
1	C	615	ASP	2.2
1	D	146	ASP	2.2
1	A	670	GLY	2.2
1	B	714	GLY	2.2
1	C	645	GLY	2.2
1	B	574	THR	2.2
1	C	575	PRO	2.2
1	B	643	ASP	2.2
1	B	578	ASP	2.2
1	A	32	GLU	2.1
1	B	610	GLU	2.1
1	B	728	PHE	2.1
1	C	730	ASP	2.1
1	A	572	ASN	2.1
1	B	616	LEU	2.1
1	C	644	ASP	2.1
1	C	720	GLU	2.1
1	A	713	GLN	2.1
1	B	723	SER	2.1
1	D	595	ASP	2.1
1	D	749	ASP	2.1
1	C	701	ALA	2.1
1	D	714	GLY	2.1
1	B	644	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	703	LYS	2.1
1	A	61	ARG	2.0
1	D	571	LEU	2.0
1	C	594	PRO	2.0
1	B	698	ALA	2.0
1	C	710	ILE	2.0
1	B	566	LEU	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](#)

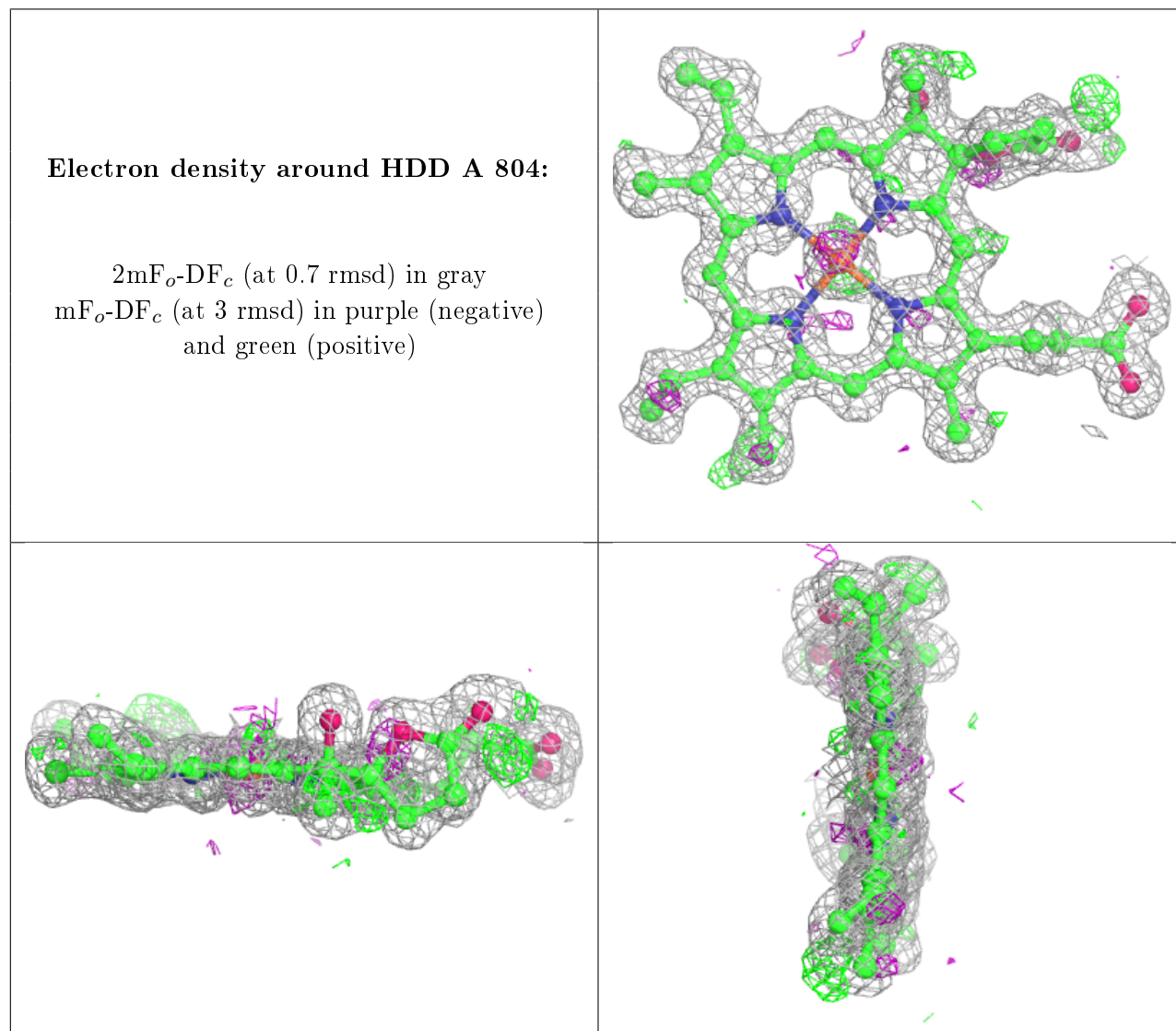
There are no monosaccharides in this entry.

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.

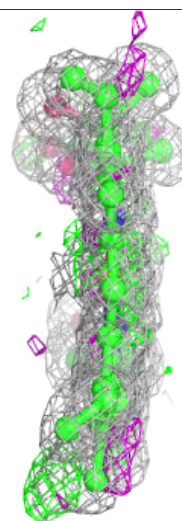
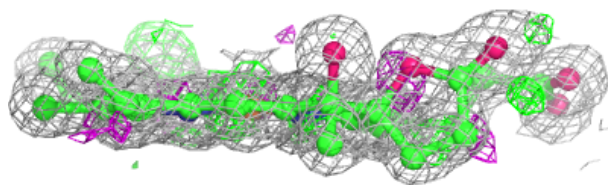
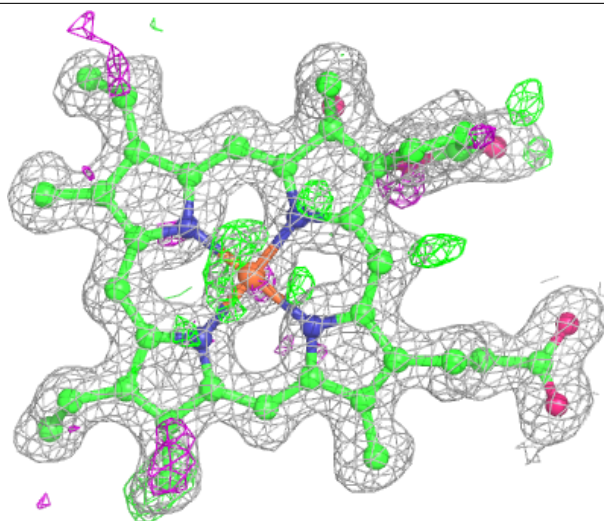
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	A	802	4/4	0.63	0.20	51,52,52,52	0
3	EDO	B	802	4/4	0.71	0.18	34,35,35,36	0
3	EDO	D	1201	4/4	0.75	0.15	33,34,34,35	0
3	EDO	A	803	4/4	0.76	0.17	29,30,30,31	0
2	GOL	A	801	6/6	0.77	0.15	20,21,23,24	0
3	EDO	D	1203	4/4	0.80	0.13	44,45,46,47	0
3	EDO	B	803	4/4	0.81	0.12	32,34,35,35	0
3	EDO	C	802	4/4	0.81	0.13	31,31,31,32	0
2	GOL	B	801	6/6	0.91	0.12	19,23,25,25	0
2	GOL	D	1202	6/6	0.92	0.09	16,20,21,21	0
2	GOL	C	801	6/6	0.97	0.06	17,19,20,21	0
4	HDD	A	804	44/44	0.98	0.09	8,10,16,17	0
4	HDD	B	804	44/44	0.98	0.09	9,11,17,18	0
4	HDD	C	803	44/44	0.98	0.08	9,11,16,17	0
4	HDD	D	1204	44/44	0.98	0.09	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.



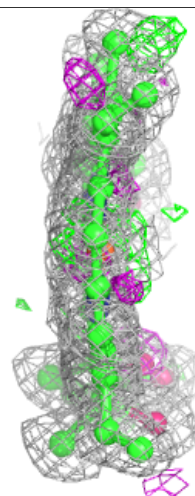
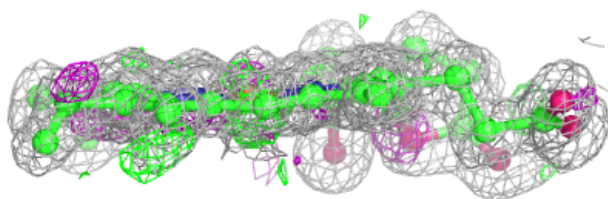
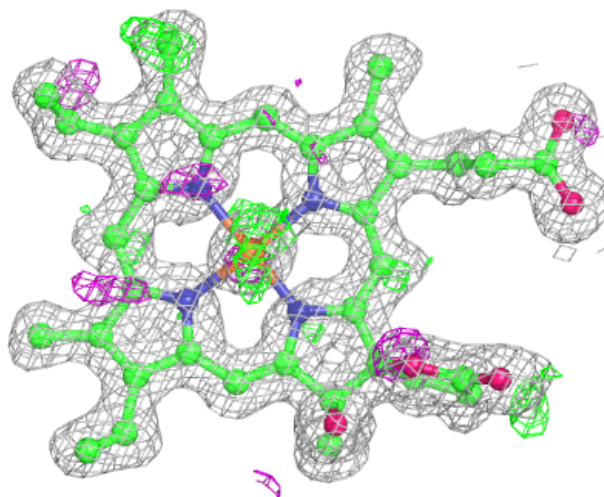
Electron density around HDD B 804:

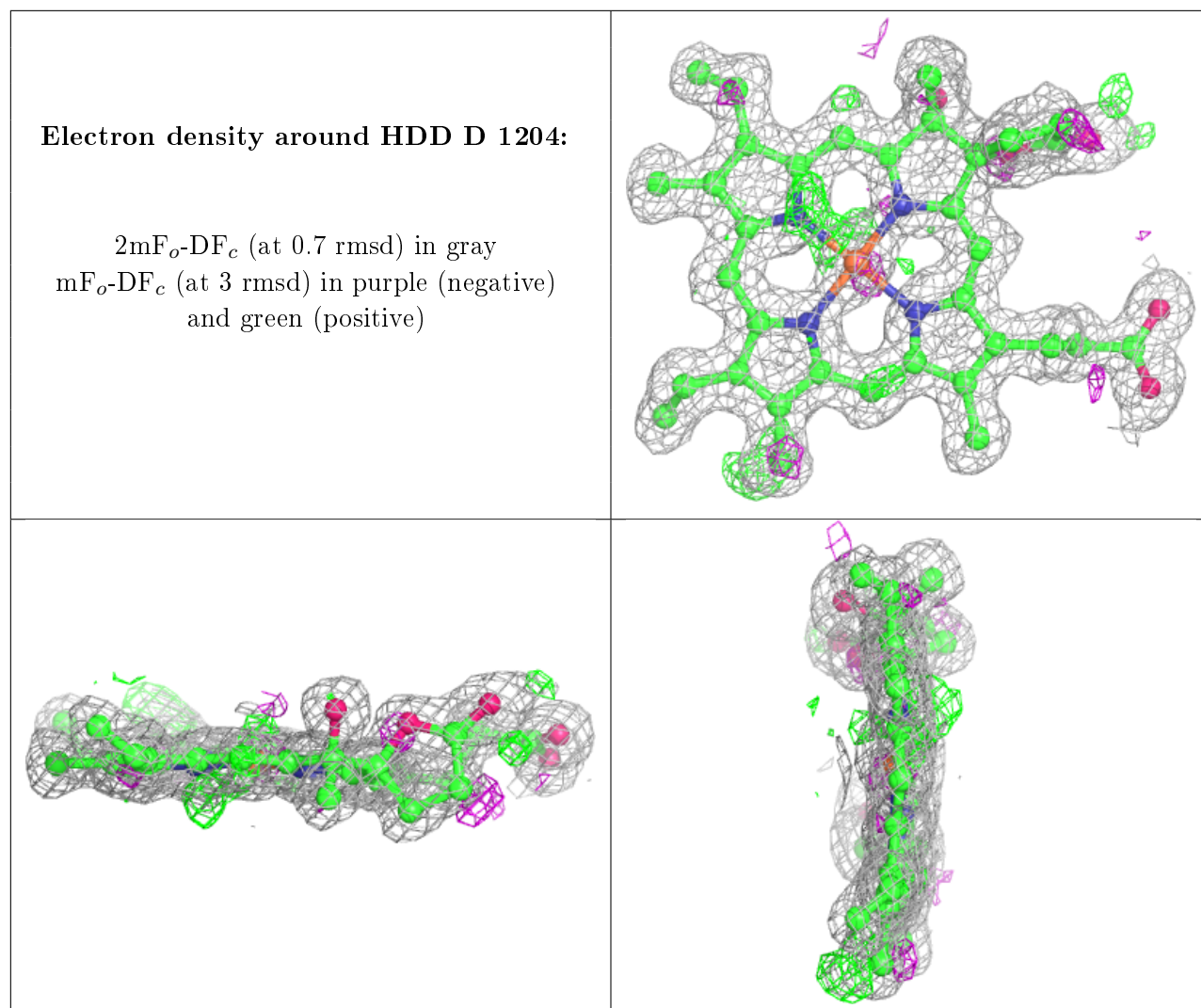
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HDD 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.