



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2021 – 07:49 PM EST

PDB ID : 1U75
Title : Electron Transfer Complex between Horse Heart Cytochrome c and Zinc-Porphyrin Substituted Cytochrome c Peroxidase
Authors : Crane, B.R.; Kang, S.A.
Deposited on : 2004-08-02
Resolution : 2.55 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
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

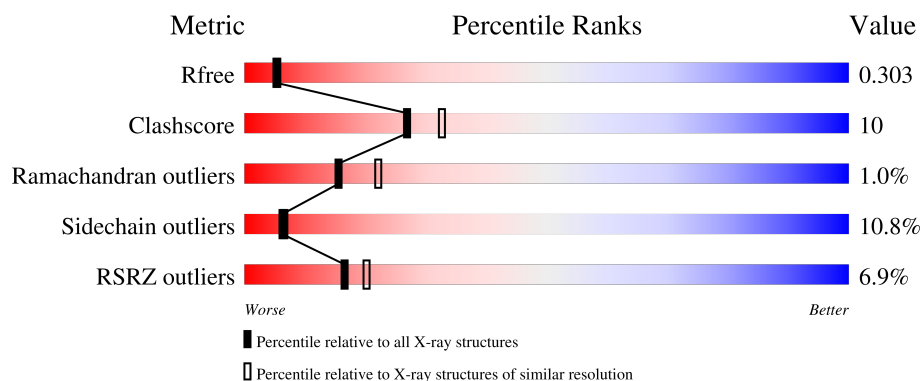
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


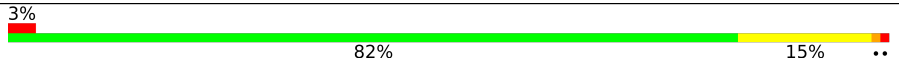
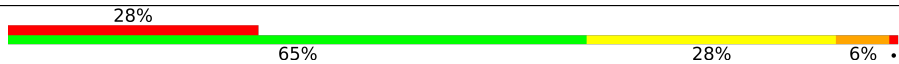
The reported resolution of this entry is 2.55 Å.

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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	296	
1	C	296	
2	B	104	

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
3	PO4	A	2201	-	-	X	-
3	PO4	C	2202	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6032 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called cytochrome c peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2371	1514	395	456	6			
1	C	295	Total	C	N	O	S	0	0	0
			2379	1520	396	457	6			

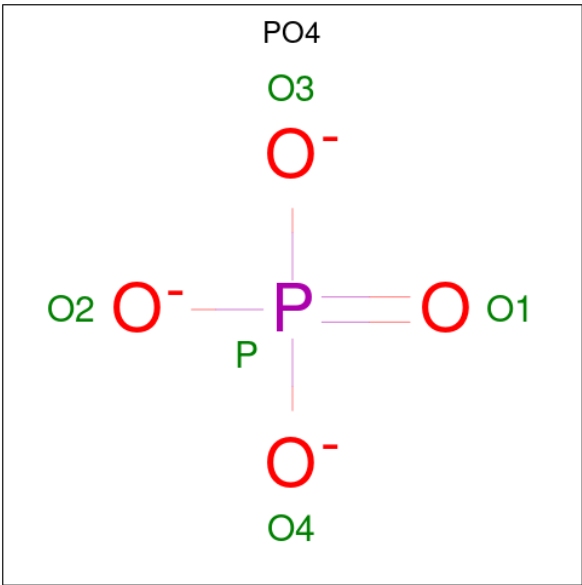
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	cloning artifact	GB 171177
A	0	ILE	-	cloning artifact	GB 171177
C	-1	MET	-	cloning artifact	GB 171177
C	0	ILE	-	cloning artifact	GB 171177

- Molecule 2 is a protein called Cytochrome c.

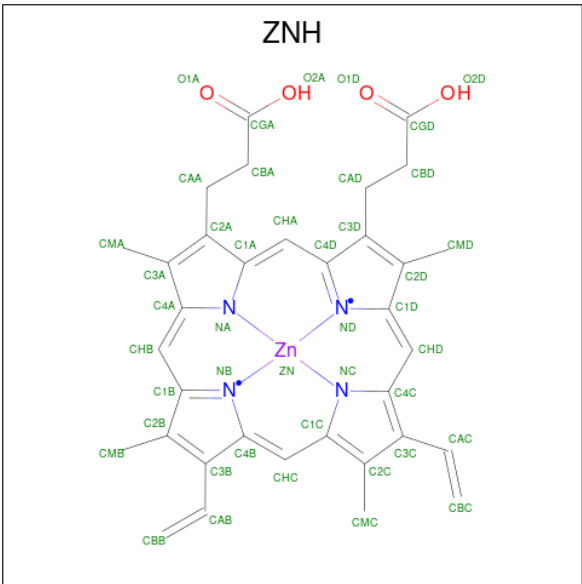
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	104	Total	C	N	O	S	0	0	0
			823	524	144	151	4			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING ZN (three-letter code: ZNH) (formula: C₃₄H₃₂N₄O₄Zn).



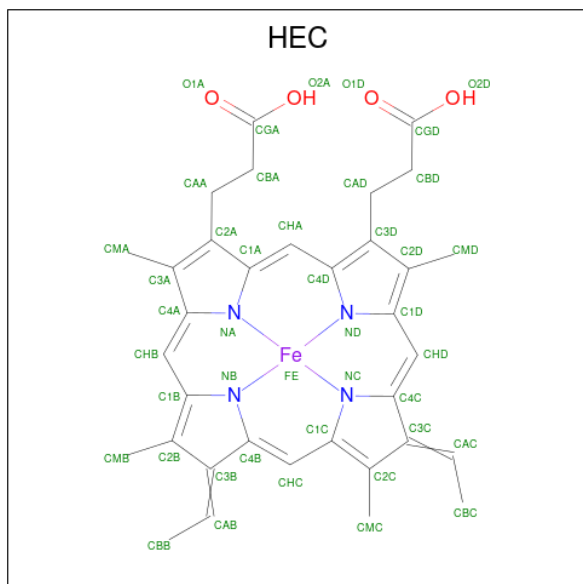
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	Zn	0	0
			43	34	4	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	Zn	0	0
			43	34	4	4	1		

- Molecule 5 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

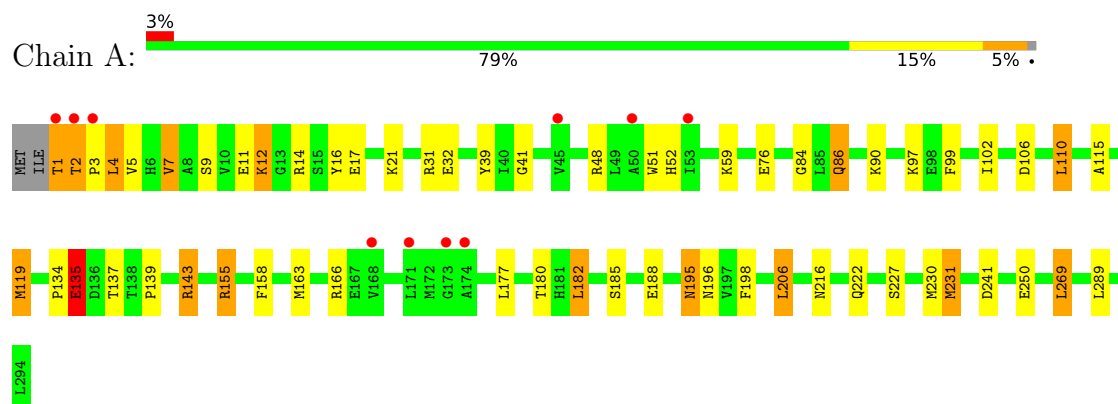
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	135	Total	O	0	0
			135	135		
6	B	45	Total	O	0	0
			45	45		
6	C	140	Total	O	0	0
			140	140		

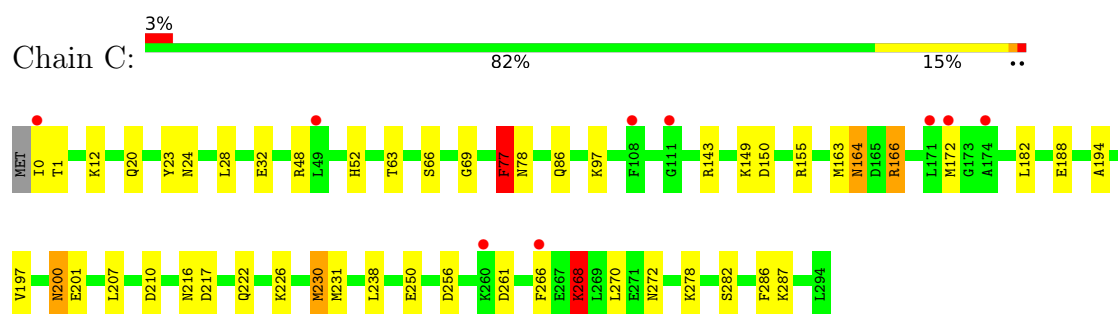
3 Residue-property plots [i](#)

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

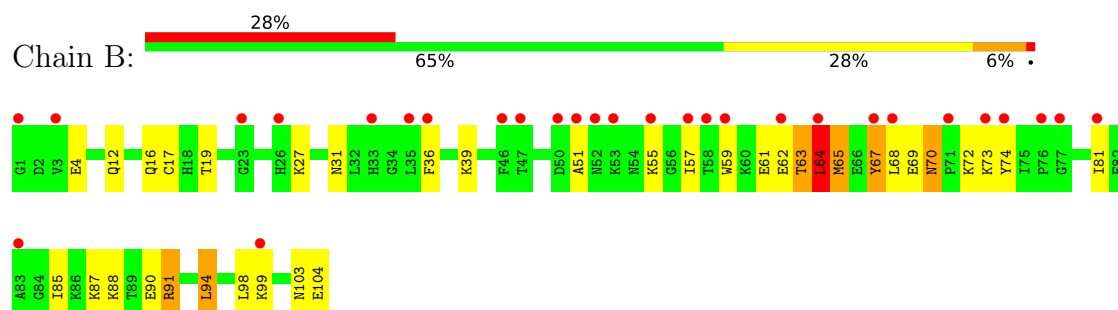
- Molecule 1: cytochrome c peroxidase



- Molecule 1: cytochrome c peroxidase



- Molecule 2: Cytochrome c



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.47Å 104.47Å 186.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.55 28.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.55) 98.6 (28.63-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.271 , 0.306 0.266 , 0.303	Depositor DCC
R_{free} test set	1786 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6032	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZNH, HEC, PO4

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	0.80	3/2438 (0.1%)	0.88	7/3302 (0.2%)
1	C	0.75	0/2446	0.85	3/3313 (0.1%)
2	B	0.85	0/839	1.10	3/1118 (0.3%)
All	All	0.79	3/5723 (0.1%)	0.90	13/7733 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	THR	C-N	7.70	1.48	1.34
1	A	1	THR	C-O	6.10	1.34	1.23
1	A	2	THR	C-O	5.70	1.34	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	THR	C-N-CD	-11.89	94.44	120.60
1	A	2	THR	C-N-CA	8.71	158.58	122.00
2	B	64	LEU	CA-CB-CG	6.53	130.31	115.30
1	C	77	PHE	CB-CG-CD1	6.03	125.02	120.80
1	A	155	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	C	77	PHE	CB-CG-CD2	-5.84	116.71	120.80
2	B	63	THR	N-CA-CB	5.51	120.77	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	155	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	268	LYS	CB-CA-C	5.22	120.84	110.40
2	B	94	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	206	LEU	CA-CB-CG	5.04	126.88	115.30
1	A	2	THR	N-CA-CB	-5.03	100.75	110.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	63	THR	Mainchain
2	B	67	TYR	Sidechain

5.2 Too-close contacts ⓘ

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	2371	0	2252	46	0
1	C	2379	0	2263	31	0
2	B	823	0	846	30	0
3	A	5	0	0	2	0
3	C	5	0	0	9	0
4	A	43	0	30	6	0
4	C	43	0	30	5	0
5	B	43	0	31	4	0
6	A	135	0	0	17	2
6	B	45	0	0	1	0
6	C	140	0	0	11	2
All	All	6032	0	5452	114	2

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 10.

All (114) 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)
2:B:17:CYS:SG	5:B:1101:HEC:HBC2	1.48	1.53
2:B:69:GLU:HB2	2:B:91:ARG:NH2	1.54	1.20
2:B:17:CYS:SG	5:B:1101:HEC:CBC	2.39	1.11
1:C:172:MET:HE2	6:C:1986:HOH:O	1.53	1.08
2:B:69:GLU:CB	2:B:91:ARG:HH22	1.68	1.05
2:B:69:GLU:CB	2:B:91:ARG:NH2	2.21	1.04
2:B:68:LEU:HB3	2:B:91:ARG:CD	1.89	1.01
1:A:31:ARG:HD3	6:A:2009:HOH:O	1.64	0.96
2:B:69:GLU:HB2	2:B:91:ARG:HH22	0.79	0.96
1:A:195:ASN:HD22	1:A:195:ASN:H	0.94	0.94
1:C:155:ARG:HD2	6:C:1987:HOH:O	1.67	0.92
1:A:84:GLY:H	1:A:86:GLN:HE22	1.15	0.88
1:C:0:ILE:HG22	1:C:1:THR:H	1.39	0.88
1:A:195:ASN:H	1:A:195:ASN:ND2	1.72	0.88
1:A:195:ASN:HD22	1:A:195:ASN:N	1.73	0.86
1:A:143:ARG:HB2	6:A:2011:HOH:O	1.77	0.84
3:C:2202:PO4:O3	4:C:1201:ZNH:NA	2.10	0.82
1:A:84:GLY:H	1:A:86:GLN:NE2	1.80	0.79
2:B:70:ASN:HB3	2:B:73:LYS:HB3	1.63	0.79
2:B:68:LEU:HD23	2:B:91:ARG:HD2	1.65	0.78
1:C:66:SER:N	6:C:1998:HOH:O	2.16	0.77
3:C:2202:PO4:O3	4:C:1201:ZNH:C1A	2.32	0.77
1:A:7:VAL:CG2	6:A:2002:HOH:O	2.33	0.77
1:A:182:LEU:HD23	6:A:2008:HOH:O	1.84	0.77
2:B:68:LEU:HB3	2:B:91:ARG:HD3	1.67	0.76
1:A:7:VAL:HG22	6:A:2002:HOH:O	1.87	0.75
1:C:200:ASN:HD22	1:C:200:ASN:H	1.33	0.75
1:A:135:GLU:OE1	6:A:2012:HOH:O	2.05	0.72
1:C:52:HIS:NE2	3:C:2202:PO4:O4	2.23	0.72
1:C:69:GLY:HA2	6:C:1991:HOH:O	1.89	0.72
1:C:238:LEU:HD21	6:C:1986:HOH:O	1.89	0.71
4:A:1001:ZNH:C3A	6:A:2004:HOH:O	2.39	0.70
1:C:20:GLN:HE22	1:C:287:LYS:H	1.39	0.70
2:B:55:LYS:HD3	2:B:57:ILE:HG12	1.74	0.70
1:A:188:GLU:H	1:A:222:GLN:HE22	1.40	0.69
2:B:68:LEU:HB3	2:B:91:ARG:HD2	1.74	0.67
1:C:216:ASN:HD22	1:C:222:GLN:NE2	1.92	0.67
1:C:52:HIS:CD2	3:C:2202:PO4:O4	2.48	0.67
1:C:48:ARG:HG3	3:C:2202:PO4:O4	1.95	0.66
1:A:216:ASN:HD22	1:A:222:GLN:HE21	1.44	0.65
1:A:216:ASN:HD22	1:A:222:GLN:NE2	1.94	0.65
2:B:64:LEU:HA	2:B:67:TYR:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:LEU:HB3	2:B:91:ARG:NE	2.16	0.60
2:B:69:GLU:CA	2:B:91:ARG:NH2	2.64	0.60
1:C:143:ARG:HB2	6:C:1990:HOH:O	2.01	0.60
1:A:185:SER:HB3	4:A:1001:ZNH:HBA1	1.84	0.60
1:A:182:LEU:CD2	6:A:2008:HOH:O	2.45	0.59
1:A:16:TYR:HD2	6:A:1836:HOH:O	1.84	0.58
1:C:238:LEU:CD2	6:C:1986:HOH:O	2.50	0.58
1:C:238:LEU:CG	6:C:1986:HOH:O	2.52	0.57
2:B:64:LEU:O	2:B:68:LEU:HB2	2.04	0.57
1:C:164:ASN:HD22	1:C:166:ARG:H	1.53	0.56
1:A:99:PHE:HD2	6:A:1522:HOH:O	1.89	0.55
2:B:17:CYS:SG	5:B:1101:HEC:CAC	2.94	0.55
3:C:2202:PO4:O3	4:C:1201:ZNH:C4A	2.55	0.54
1:C:238:LEU:HG	6:C:1986:HOH:O	2.08	0.54
1:A:155:ARG:HH22	1:A:241:ASP:CG	2.11	0.54
3:C:2202:PO4:O2	4:C:1201:ZNH:C1B	2.55	0.54
1:A:134:PRO:O	1:A:137:THR:HG22	2.08	0.54
1:A:17:GLU:HG3	6:A:1836:HOH:O	2.07	0.53
1:A:41:GLY:CA	6:A:2013:HOH:O	2.55	0.53
1:C:23:TYR:HD1	1:C:24:ASN:HD22	1.56	0.52
1:C:182:LEU:HB2	1:C:188:GLU:HG2	1.92	0.52
2:B:87:LYS:O	2:B:91:ARG:HG3	2.10	0.51
1:C:77:PHE:HB3	1:C:78:ASN:HD22	1.75	0.51
1:A:7:VAL:HG23	6:A:2002:HOH:O	2.06	0.51
1:A:76:GLU:CG	6:A:2010:HOH:O	2.59	0.50
1:C:77:PHE:HB3	1:C:78:ASN:ND2	2.27	0.50
3:C:2202:PO4:O2	4:C:1201:ZNH:NB	2.44	0.50
1:A:97:LYS:HE3	6:A:1989:HOH:O	2.10	0.50
1:A:48:ARG:HD2	4:A:1001:ZNH:HBD1	1.94	0.50
1:A:11:GLU:O	1:A:14:ARG:HB2	2.12	0.49
1:A:52:HIS:NE2	3:A:2201:PO4:P	2.86	0.49
1:C:0:ILE:HG22	1:C:1:THR:N	2.19	0.49
1:A:206:LEU:HD13	1:A:231:MET:HG2	1.94	0.49
1:C:272:ASN:HB2	6:C:2000:HOH:O	2.12	0.49
1:A:4:LEU:H	1:A:4:LEU:HD23	1.78	0.49
1:C:0:ILE:CG2	1:C:1:THR:H	2.18	0.49
1:C:266:PHE:O	1:C:270:LEU:HG	2.14	0.48
1:A:4:LEU:HD23	1:A:4:LEU:N	2.28	0.48
1:A:216:ASN:ND2	1:A:222:GLN:HE21	2.10	0.48
1:A:52:HIS:CD2	3:A:2201:PO4:O1	2.67	0.47
4:A:1001:ZNH:C2A	6:A:2004:HOH:O	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:PHE:HD2	6:C:1996:HOH:O	1.98	0.47
1:A:139:PRO:HB2	1:A:143:ARG:HE	1.79	0.47
1:A:86:GLN:HE21	1:A:86:GLN:H	1.62	0.46
1:A:177:LEU:HD11	1:A:198:PHE:HD1	1.80	0.46
2:B:69:GLU:N	2:B:91:ARG:CZ	2.78	0.46
2:B:36:PHE:HA	2:B:59:TRP:O	2.16	0.46
2:B:68:LEU:CB	2:B:91:ARG:CD	2.79	0.44
1:A:166:ARG:HH22	1:A:250:GLU:CD	2.20	0.44
1:A:195:ASN:ND2	1:A:195:ASN:N	2.44	0.44
2:B:16:GLN:HG3	6:B:1924:HOH:O	2.17	0.44
2:B:62:GLU:HA	2:B:65:MET:HB2	1.98	0.44
1:A:166:ARG:NH2	1:A:250:GLU:OE2	2.51	0.43
1:A:115:ALA:O	1:A:119:MET:HB2	2.18	0.43
1:A:39:TYR:HE1	2:B:90:GLU:HG3	1.83	0.43
4:A:1001:ZNH:HA	4:A:1001:ZNH:HAA1	1.89	0.43
1:A:158:PHE:HB3	1:A:163:MET:HB2	2.01	0.43
2:B:36:PHE:HZ	2:B:98:LEU:HB3	1.84	0.43
2:B:68:LEU:CB	2:B:91:ARG:HD3	2.45	0.42
1:C:48:ARG:HD2	3:C:2202:PO4:O3	2.20	0.42
1:C:230:MET:HG2	1:C:231:MET:N	2.34	0.42
1:C:149:LYS:HB3	1:C:150:ASP:H	1.74	0.42
2:B:68:LEU:CD2	2:B:91:ARG:HD2	2.43	0.42
1:A:99:PHE:O	1:A:102:ILE:HG22	2.20	0.41
1:A:106:ASP:O	1:A:110:LEU:HB2	2.20	0.41
1:C:163:MET:CE	1:C:268:LYS:HG2	2.51	0.41
2:B:59:TRP:CZ2	5:B:1101:HEC:HAA1	2.56	0.41
1:A:41:GLY:HA2	6:A:2013:HOH:O	2.18	0.41
1:C:194:ALA:HB1	1:C:197:VAL:HG12	2.02	0.41
2:B:69:GLU:HA	2:B:85:ILE:O	2.21	0.41
1:A:180:THR:HG22	4:A:1001:ZNH:HAA2	2.03	0.40
2:B:69:GLU:N	2:B:91:ARG:NH2	2.69	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2017:HOH:O	6:C:1999:HOH:O[8_565]	0.59	1.61
6:A:2015:HOH:O	6:C:1401:HOH:O[8_565]	0.60	1.60

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	292/296 (99%)	277 (95%)	11 (4%)	4 (1%)	11	15
1	C	293/296 (99%)	281 (96%)	11 (4%)	1 (0%)	41	51
2	B	102/104 (98%)	90 (88%)	10 (10%)	2 (2%)	7	8
All	All	687/696 (99%)	648 (94%)	32 (5%)	7 (1%)	15	22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	64	LEU
2	B	51	ALA
1	A	12	LYS
1	C	12	LYS
1	A	3	PRO
1	A	135	GLU

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	252/254 (99%)	228 (90%)	24 (10%)	8	10
1	C	253/254 (100%)	232 (92%)	21 (8%)	11	14
2	B	86/86 (100%)	67 (78%)	19 (22%)	1	1
All	All	591/594 (100%)	527 (89%)	64 (11%)	6	6

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	4	LEU
1	A	5	VAL
1	A	7	VAL
1	A	9	SER
1	A	12	LYS
1	A	21	LYS
1	A	32	GLU
1	A	51	TRP
1	A	59	LYS
1	A	86	GLN
1	A	90	LYS
1	A	110	LEU
1	A	119	MET
1	A	135	GLU
1	A	143	ARG
1	A	182	LEU
1	A	195	ASN
1	A	196	ASN
1	A	227	SER
1	A	230	MET
1	A	231	MET
1	A	269	LEU
1	A	289	LEU
2	B	4	GLU
2	B	12	GLN
2	B	19	THR
2	B	27	LYS
2	B	31	ASN
2	B	39	LYS
2	B	61	GLU
2	B	64	LEU
2	B	65	MET
2	B	70	ASN
2	B	72	LYS
2	B	74	TYR
2	B	81	ILE
2	B	88	LYS
2	B	91	ARG
2	B	94	LEU
2	B	99	LYS
2	B	103	ASN

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Mol	Chain	Res	Type
2	B	104	GLU
1	C	28	LEU
1	C	32	GLU
1	C	63	THR
1	C	77	PHE
1	C	86	GLN
1	C	97	LYS
1	C	164	ASN
1	C	166	ARG
1	C	200	ASN
1	C	201	GLU
1	C	207	LEU
1	C	210	ASP
1	C	217	ASP
1	C	226	LYS
1	C	230	MET
1	C	250	GLU
1	C	256	ASP
1	C	261	ASP
1	C	268	LYS
1	C	278	LYS
1	C	282	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	86	GLN
1	A	96	HIS
1	A	195	ASN
1	A	196	ASN
1	A	222	GLN
1	A	292	GLN
2	B	12	GLN
2	B	54	ASN
1	C	20	GLN
1	C	24	ASN
1	C	78	ASN
1	C	117	GLN
1	C	159	GLN
1	C	164	ASN
1	C	200	ASN

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Mol	Chain	Res	Type
1	C	208	ASN
1	C	222	GLN
1	C	240	GLN
1	C	292	GLN

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](#)

5 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	$\# Z > 2$
4	ZNH	C	1201	1,3	35,50,50	4.60	23 (65%)	18,82,82	2.43	8 (44%)
3	PO4	A	2201	4,1	4,4,4	3.78	1 (25%)	6,6,6	1.79	2 (33%)
3	PO4	C	2202	4	4,4,4	2.49	1 (25%)	6,6,6	1.39	2 (33%)
5	HEC	B	1101	2	26,50,50	1.65	5 (19%)	18,82,82	1.93	6 (33%)
4	ZNH	A	1001	1,3	35,50,50	4.97	23 (65%)	18,82,82	3.02	7 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEC	B	1101	2	-	1/6/54/54	-
4	ZNH	A	1001	1,3	-	0/8/94/94	-
4	ZNH	C	1201	1,3	-	0/8/94/94	-

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	ZNH	CHA-C4D	-9.88	1.36	1.53
4	A	1001	ZNH	CHC-C4B	-9.33	1.37	1.53
4	A	1001	ZNH	CHB-C1B	-8.24	1.39	1.53
4	C	1201	ZNH	CHC-C4B	-8.23	1.39	1.53
4	A	1001	ZNH	C4B-NB	-8.20	1.35	1.49
4	C	1201	ZNH	C4D-ND	-8.17	1.35	1.49
4	A	1001	ZNH	C4D-ND	-8.11	1.35	1.49
4	A	1001	ZNH	CHD-C1D	-8.05	1.39	1.53
4	C	1201	ZNH	CHB-C1B	-8.05	1.39	1.53
4	C	1201	ZNH	CHD-C1D	-7.70	1.40	1.53
4	A	1001	ZNH	C1B-NB	-7.57	1.36	1.49
4	A	1001	ZNH	C1D-ND	-7.55	1.36	1.49
4	C	1201	ZNH	CHA-C4D	-7.36	1.40	1.53
3	A	2201	PO4	P-O1	7.30	1.68	1.50
4	C	1201	ZNH	C4B-NB	-7.17	1.37	1.49
4	A	1001	ZNH	C4A-C3A	6.87	1.47	1.38
4	C	1201	ZNH	C1D-ND	-6.72	1.38	1.49
4	C	1201	ZNH	C1B-NB	-6.40	1.38	1.49
4	C	1201	ZNH	CHB-C4A	-6.10	1.36	1.51
4	C	1201	ZNH	C4A-C3A	5.85	1.46	1.38
4	C	1201	ZNH	C1A-C2A	5.70	1.45	1.38
4	A	1001	ZNH	CHA-C1A	-5.58	1.37	1.51
4	A	1001	ZNH	CHC-C1C	-5.57	1.37	1.51
4	C	1201	ZNH	C1C-C2C	5.00	1.45	1.38
4	A	1001	ZNH	C1A-C2A	4.84	1.44	1.38
4	A	1001	ZNH	CHB-C4A	-4.56	1.40	1.51
4	C	1201	ZNH	CHA-C1A	-4.52	1.40	1.51
4	C	1201	ZNH	C1C-NC	4.48	1.39	1.34
3	C	2202	PO4	P-O2	4.47	1.68	1.54
4	C	1201	ZNH	C4A-NA	4.43	1.39	1.34
4	A	1001	ZNH	C1C-C2C	4.37	1.44	1.38
4	C	1201	ZNH	CHD-C4C	-4.29	1.40	1.51
4	C	1201	ZNH	CHC-C1C	-4.26	1.40	1.51
4	A	1001	ZNH	C4C-NC	4.14	1.39	1.34
4	A	1001	ZNH	CHD-C4C	-4.06	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	ZNH	C3C-CAC	-3.88	1.40	1.47
4	C	1201	ZNH	C2D-C3D	3.85	1.37	1.34
4	A	1001	ZNH	C2D-C3D	3.78	1.37	1.34
4	C	1201	ZNH	C4B-C3B	-3.51	1.45	1.51
4	A	1001	ZNH	CAD-C3D	3.43	1.56	1.51
4	C	1201	ZNH	C3C-CAC	-3.39	1.41	1.47
5	B	1101	HEC	C3B-C2B	-3.30	1.37	1.40
4	A	1001	ZNH	CMB-C2B	3.23	1.55	1.50
4	A	1001	ZNH	C4B-C3B	-3.20	1.46	1.51
5	B	1101	HEC	CBB-CAB	-3.20	1.37	1.49
5	B	1101	HEC	C4D-CHA	-3.08	1.32	1.41
5	B	1101	HEC	C3C-C4C	3.04	1.48	1.43
4	A	1001	ZNH	C3C-C2C	-2.93	1.36	1.40
4	C	1201	ZNH	CAD-C3D	2.75	1.55	1.51
5	B	1101	HEC	C3B-C4B	2.55	1.47	1.43
4	A	1001	ZNH	C4A-NA	2.22	1.36	1.34
4	C	1201	ZNH	C1A-NA	2.22	1.36	1.34
4	C	1201	ZNH	C4C-NC	2.19	1.36	1.34

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	ZNH	CAA-C2A-C1A	-9.00	120.98	127.30
5	B	1101	HEC	C1D-C2D-C3D	-5.52	103.16	107.00
4	A	1001	ZNH	C3C-C4C-NC	5.43	111.28	107.55
4	C	1201	ZNH	CBA-CAA-C2A	4.95	121.61	112.49
4	C	1201	ZNH	C3C-C4C-NC	4.83	110.86	107.55
4	A	1001	ZNH	CBA-CAA-C2A	3.80	119.49	112.49
4	C	1201	ZNH	CMC-C2C-C3C	3.49	131.21	124.68
4	C	1201	ZNH	CHB-C4A-C3A	-3.38	123.60	129.45
4	C	1201	ZNH	CHD-C4C-C3C	-2.87	125.69	129.55
4	A	1001	ZNH	CMC-C2C-C3C	2.73	129.78	124.68
4	A	1001	ZNH	CHC-C1C-C2C	-2.72	124.74	129.45
4	C	1201	ZNH	CHC-C1C-C2C	-2.67	124.82	129.45
5	B	1101	HEC	CMA-C3A-C2A	2.67	129.97	124.94
3	A	2201	PO4	O3-P-O1	-2.62	101.29	110.89
5	B	1101	HEC	CBA-CAA-C2A	2.44	116.97	112.48
3	A	2201	PO4	O4-P-O3	2.42	115.75	107.97
3	C	2202	PO4	O4-P-O3	2.42	115.75	107.97
4	C	1201	ZNH	CAA-C2A-C1A	-2.30	125.68	127.30
4	A	1001	ZNH	CMA-C3A-C2A	2.29	129.26	124.94
4	C	1201	ZNH	C4A-C3A-C2A	-2.29	103.37	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1101	HEC	CMB-C2B-C1B	-2.22	125.06	128.46
5	B	1101	HEC	CMD-C2D-C1D	2.20	131.84	128.46
5	B	1101	HEC	CMB-C2B-C3B	2.13	128.32	125.82
4	A	1001	ZNH	CAA-C2A-C3A	2.10	133.28	127.25
3	C	2202	PO4	O3-P-O2	-2.08	101.30	107.97

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1101	HEC	C3A-C2A-CAA-CBA

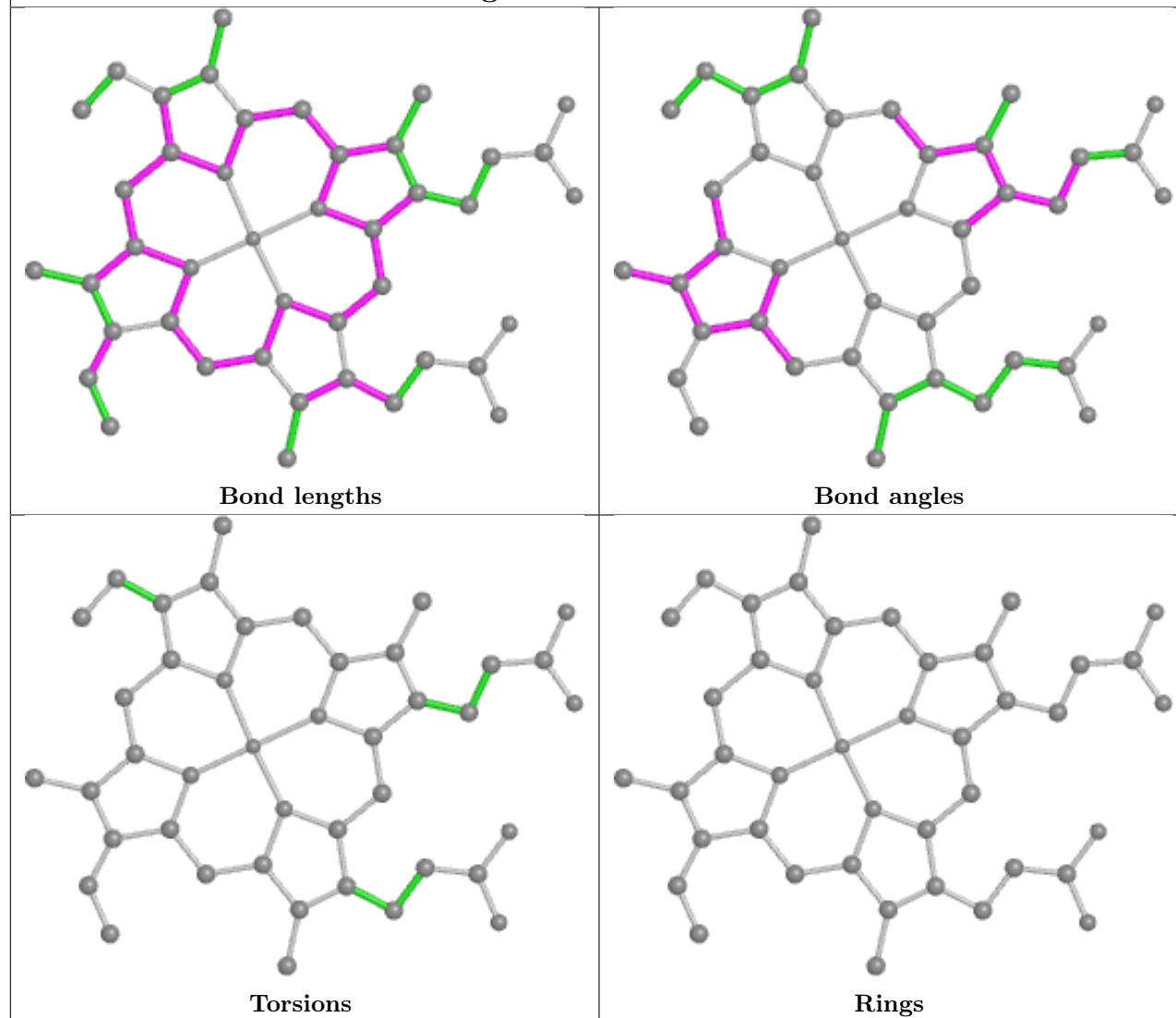
There are no ring outliers.

5 monomers are involved in 21 short contacts:

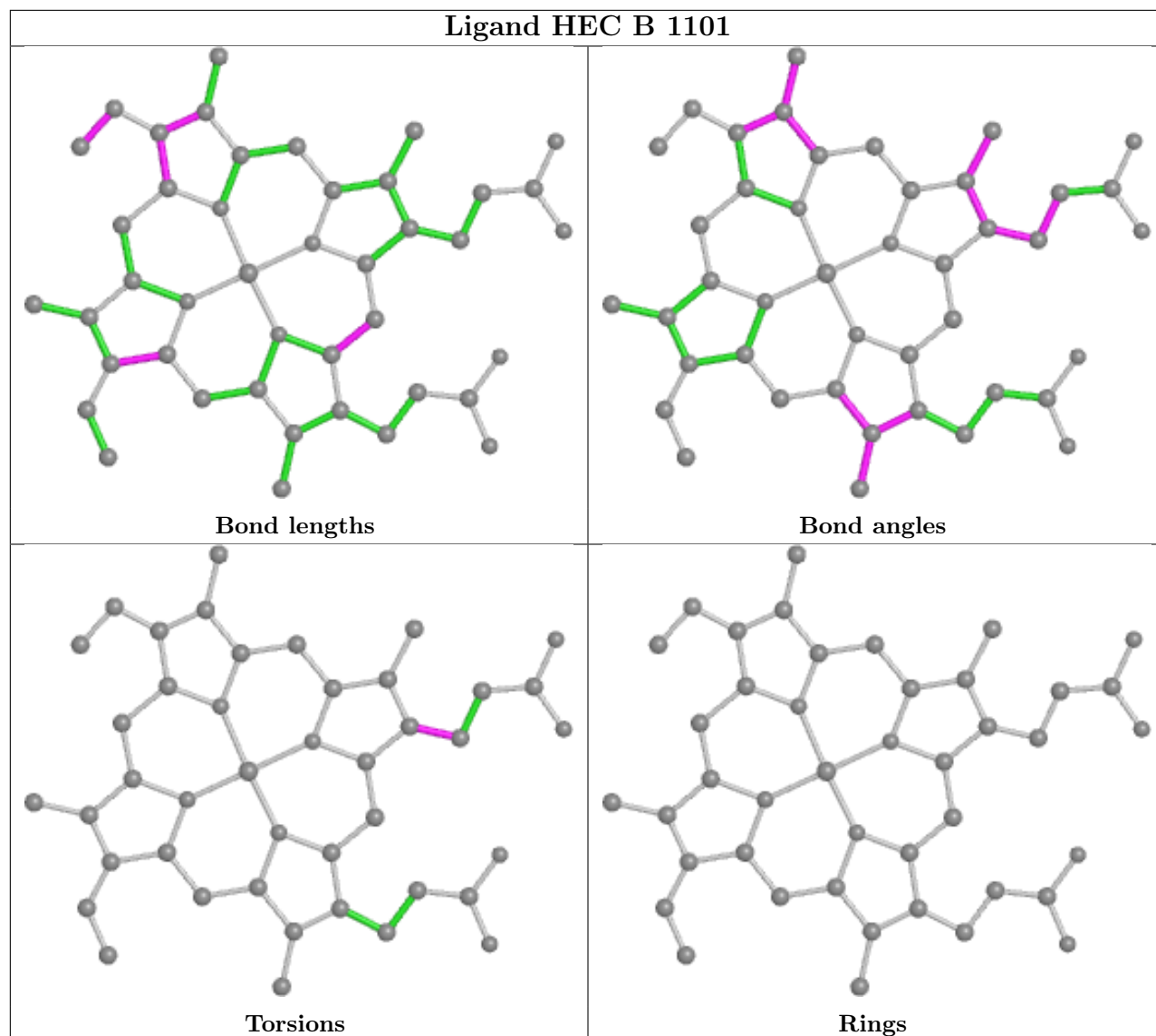
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1201	ZNH	5	0
3	A	2201	PO4	2	0
3	C	2202	PO4	9	0
5	B	1101	HEC	4	0
4	A	1001	ZNH	6	0

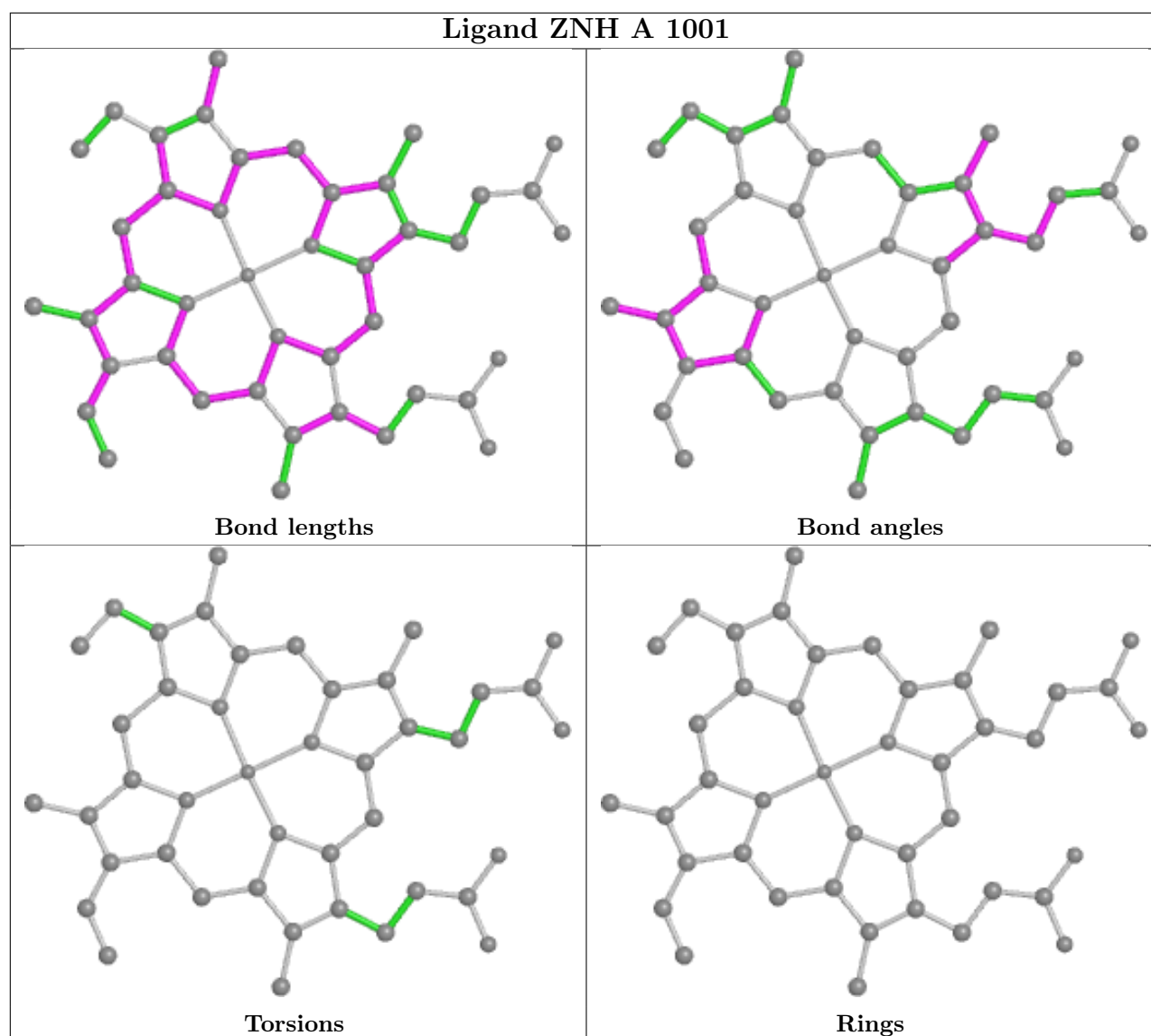
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand ZNH C 1201



Ligand HEC B 1101





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	294/296 (99%)	0.10	10 (3%) 45 52	46, 56, 69, 101	0
1	C	295/296 (99%)	0.12	9 (3%) 49 56	45, 57, 67, 87	0
2	B	104/104 (100%)	1.49	29 (27%) 0 0	40, 62, 72, 75	0
All	All	693/696 (99%)	0.31	48 (6%) 16 20	40, 57, 70, 101	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	THR	9.0
2	B	36	PHE	7.8
1	A	2	THR	7.7
2	B	51	ALA	6.7
2	B	3	VAL	4.7
2	B	74	TYR	4.4
2	B	23	GLY	4.3
1	C	0	ILE	4.0
2	B	64	LEU	4.0
2	B	33	HIS	3.8
2	B	50	ASP	3.7
1	C	174	ALA	3.6
2	B	83	ALA	3.6
2	B	46	PHE	3.6
2	B	47	THR	3.5
2	B	68	LEU	3.5
2	B	62	GLU	3.4
2	B	57	ILE	3.4
2	B	59	TRP	3.4
2	B	26	HIS	3.4
1	A	3	PRO	3.4
1	C	171	LEU	3.3
1	C	49	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	73	LYS	3.2
2	B	67	TYR	3.1
2	B	81	ILE	3.1
1	A	168	VAL	3.1
2	B	1	GLY	3.0
1	C	260	LYS	2.9
1	A	174	ALA	2.8
1	A	50	ALA	2.8
2	B	55	LYS	2.8
1	C	111	GLY	2.7
1	A	171	LEU	2.7
2	B	35	LEU	2.7
2	B	52	ASN	2.6
2	B	99	LYS	2.6
1	C	266	PHE	2.5
2	B	58	THR	2.4
1	A	53	ILE	2.4
1	C	108	PHE	2.4
2	B	53	LYS	2.3
2	B	71	PRO	2.3
1	C	172	MET	2.2
2	B	77	GLY	2.2
1	A	45	VAL	2.1
2	B	76	PRO	2.1
1	A	173	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

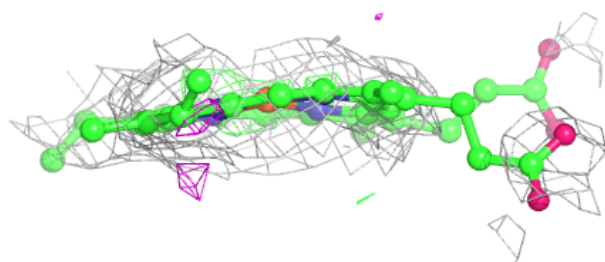
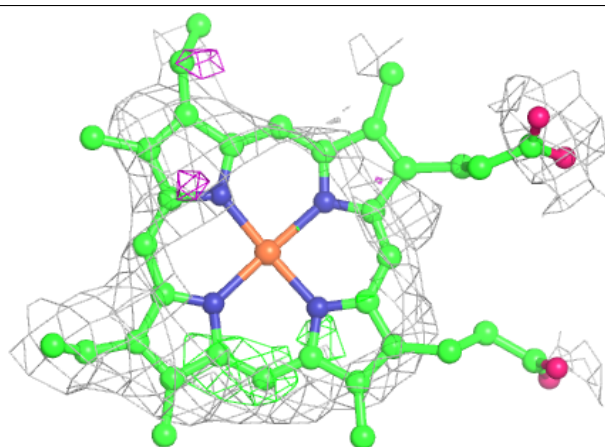
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	HEC	B	1101	43/43	0.88	0.28	45,51,59,65	0
3	PO4	A	2201	5/5	0.92	0.33	83,96,99,105	0
3	PO4	C	2202	5/5	0.93	0.24	98,106,106,114	0
4	ZNH	C	1201	43/43	0.96	0.20	47,56,60,61	0
4	ZNH	A	1001	43/43	0.96	0.17	46,54,57,65	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.

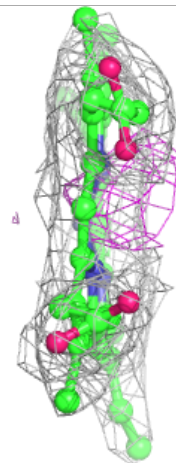
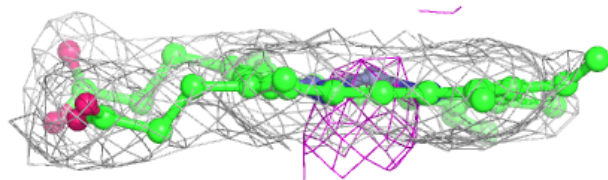
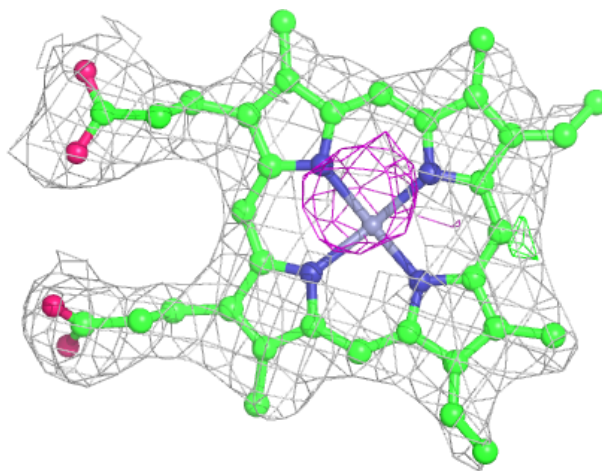
Electron density around HEC B 1101:

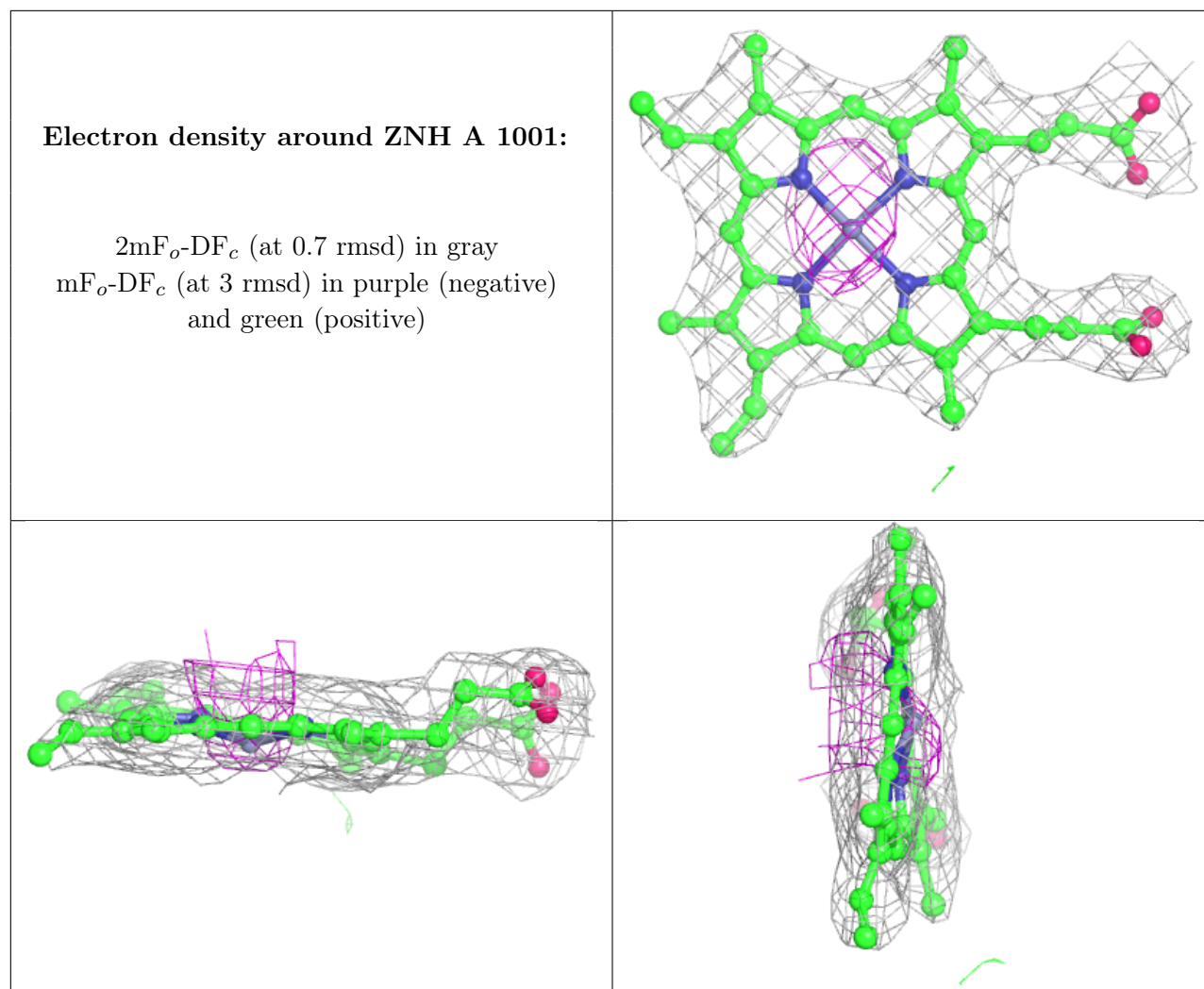
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZNH C 1201:

$2mF_o-DF_c$ (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.