



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 01:57 PM EDT

PDB ID : 1U75 / pdb_00001u75
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 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

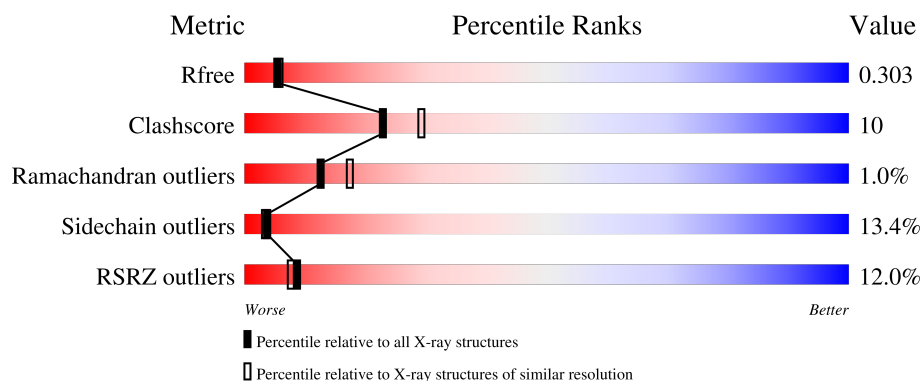
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	X
3	PO4	C	2202	-	-	X	X
4	ZNH	A	1001	X	-	-	-
4	ZNH	C	1201	X	-	-	-
5	HEC	B	1101	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.

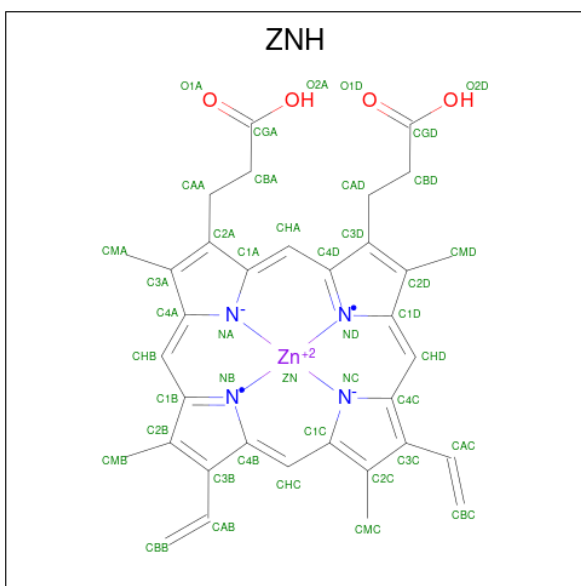
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	104	Total	C	N	O	S	0	0	0
			823	524	144	151	4			

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



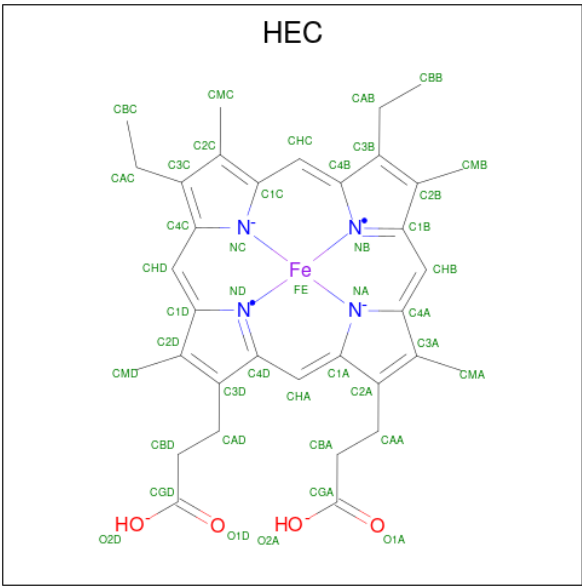
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	O	P		0	0
			5	4	1			
3	C	1	Total	O	P		0	0
			5	4	1			

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING ZN (CCD ID: ZNH) (formula: $C_{34}H_{32}N_4O_4Zn$).



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

- Molecule 5 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



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

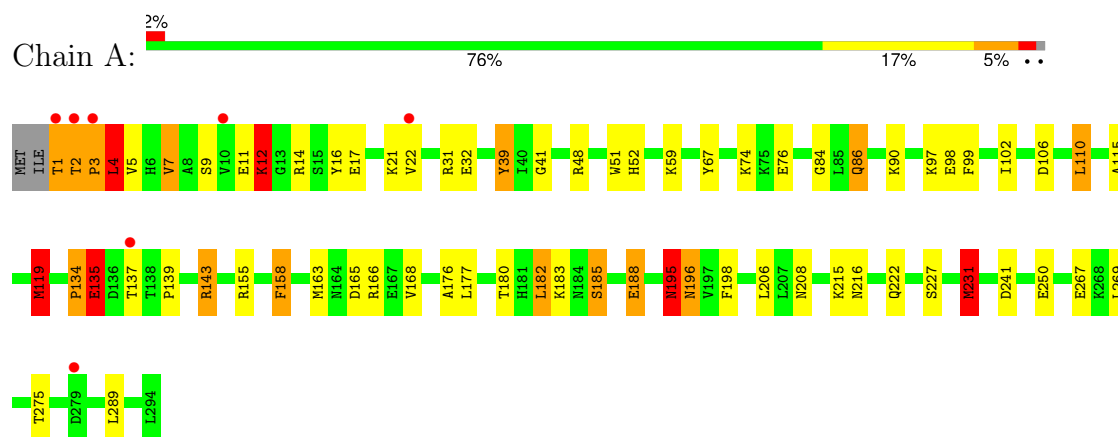
- Molecule 6 is water.

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		

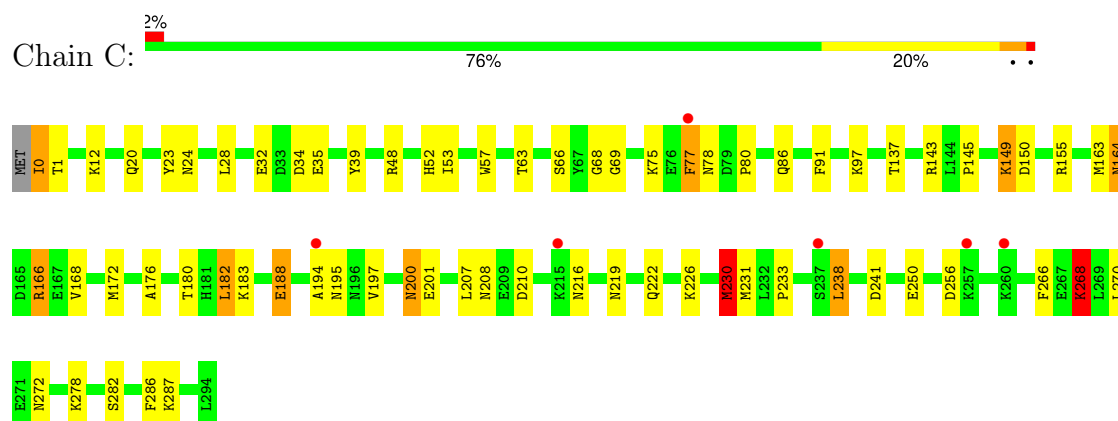
3 Residue-property plots [i](#)

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.

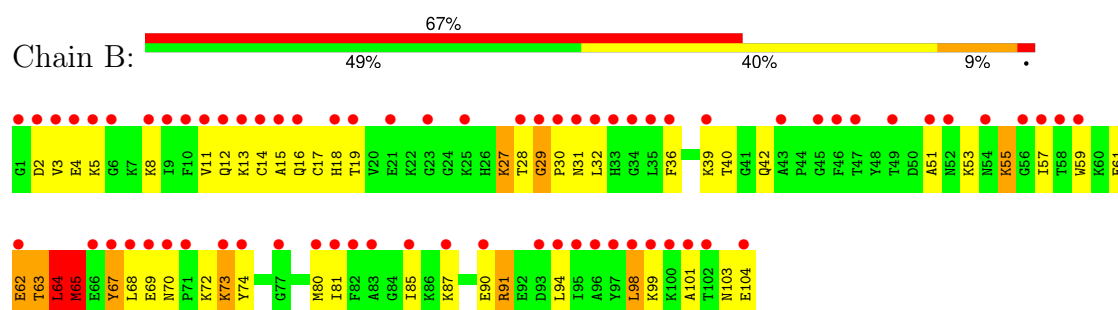
- Molecule 1: cytochrome c peroxidase



- 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 20.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.55) 98.4 (20.00-2.55)	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)	0.23 , 24.0	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	0.90	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	0.83	7/2438 (0.3%)	1.28	20/3302 (0.6%)
1	C	0.75	1/2446 (0.0%)	1.26	18/3313 (0.5%)
2	B	0.96	0/839	1.65	20/1118 (1.8%)
All	All	0.82	8/5723 (0.1%)	1.33	58/7733 (0.8%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	230	MET	SD-CE	-8.61	1.58	1.79
1	A	2	THR	C-O	7.76	1.34	1.24
1	A	2	THR	C-N	7.70	1.48	1.34
1	A	119	MET	SD-CE	-6.47	1.63	1.79
1	A	2	THR	CA-CB	6.04	1.62	1.53
1	A	231	MET	SD-CE	-6.04	1.64	1.79
1	A	1	THR	C-O	5.69	1.34	1.23
1	A	3	PRO	CB-CG	5.29	1.71	1.51

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	THR	CA-C-N	13.16	158.58	127.00
1	A	2	THR	C-N-CA	13.16	158.58	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	65	MET	N-CA-C	-12.20	98.10	113.23
1	A	2	THR	C-N-CD	-11.89	94.44	120.60
1	C	238	LEU	N-CA-C	-10.16	99.66	114.39
2	B	42	GLN	N-CA-C	9.11	122.51	111.40
1	A	74	LYS	N-CA-C	8.78	120.85	111.28
2	B	3	VAL	N-CA-C	-7.60	102.22	113.39
1	A	176	ALA	N-CA-C	-7.58	104.01	113.18
2	B	2	ASP	N-CA-C	7.38	121.20	110.42
1	A	4	LEU	N-CA-C	7.37	121.85	109.76
1	C	149	LYS	N-CA-C	6.98	119.13	109.29
2	B	18	HIS	N-CA-C	6.83	120.28	109.50
1	C	241	ASP	CA-C-N	6.72	126.68	119.28
1	C	241	ASP	C-N-CA	6.72	126.68	119.28
1	C	145	PRO	N-CA-C	6.65	121.39	111.41
1	A	2	THR	CB-CA-C	6.54	123.05	110.17
2	B	32	LEU	N-CA-C	6.32	120.67	113.15
1	C	208	ASN	N-CA-C	6.28	120.68	112.89
1	C	35	GLU	N-CA-C	6.28	121.08	113.17
1	A	208	ASN	N-CA-C	6.26	121.99	113.97
2	B	14	CYS	N-CA-C	6.21	121.44	113.18
2	B	63	THR	N-CA-CB	6.17	120.77	110.53
1	C	195	ASN	N-CA-C	6.13	119.79	112.93
1	C	39	TYR	N-CA-C	6.12	122.06	113.56
1	C	268	LYS	CB-CA-C	6.05	120.84	110.79
2	B	55	LYS	N-CA-C	-6.02	104.84	111.82
1	A	134	PRO	N-CA-C	5.97	120.71	111.21
2	B	13	LYS	N-CA-C	5.96	120.72	113.38
1	C	176	ALA	N-CA-C	-5.95	105.51	112.89
2	B	28	THR	N-CA-C	-5.90	106.72	112.97
1	C	91	PHE	N-CA-C	-5.89	104.26	112.45
1	A	98	GLU	N-CA-C	-5.86	105.22	112.90
2	B	62	GLU	CA-C-N	-5.77	114.23	122.77
2	B	62	GLU	C-N-CA	-5.77	114.23	122.77
1	A	188	GLU	N-CA-C	5.76	118.49	108.76
1	A	165	ASP	N-CA-C	5.74	118.28	111.33
2	B	15	ALA	N-CA-C	5.61	119.63	112.34
1	C	34	ASP	N-CA-C	5.59	119.84	113.19
1	C	68	GLY	N-CA-C	5.58	121.14	113.99
2	B	29	GLY	CA-C-N	5.57	125.55	120.03
2	B	29	GLY	C-N-CA	5.57	125.55	120.03
2	B	101	ALA	N-CA-C	5.52	118.06	111.71
1	A	158	PHE	N-CA-C	5.52	119.63	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	LYS	N-CA-C	-5.49	106.58	113.28
1	A	12	LYS	N-CA-C	5.47	122.45	110.80
1	C	137	THR	N-CA-C	-5.44	106.32	113.17
1	A	2	THR	N-CA-CB	-5.41	100.75	110.37
2	B	30	PRO	CB-CA-C	-5.36	103.92	110.95
2	B	53	LYS	N-CA-C	-5.28	105.69	111.82
1	C	57	TRP	N-CA-C	5.25	117.85	110.23
1	A	195	ASN	N-CA-C	5.25	119.25	113.21
1	C	182	LEU	N-CA-C	5.24	116.67	111.07
1	A	227	SER	N-CA-C	-5.23	106.29	113.30
1	A	39	TYR	N-CA-C	5.20	119.58	113.23
1	C	180	THR	N-CA-C	-5.20	101.79	110.17
1	A	185	SER	N-CA-C	5.17	119.68	112.90
1	A	67	TYR	N-CA-C	5.08	119.69	111.37

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	47	0
1	C	2379	0	2263	31	0
2	B	823	0	846	31	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6032	0	5452	116	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 (116) 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
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:C:172:MET:HE3	6:C:1986:HOH:O	1.59	1.00
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:C:163:MET:HE1	1:C:268:LYS:HG2	1.62	0.80
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:155:ARG:HH22	1:A:241:ASP:CG	2.11	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:166:ARG:HH22	1:A:250:GLU:CD	2.20	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
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:196:ASN:C	1:A:196:ASN:HD22	2.25	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:HAHA	4:A:1001:ZNH:HAA1	1.89	0.43
2:B:27:LYS:C	2:B:29:GLY:H	2.27	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	292/296 (99%)	277 (95%)	11 (4%)	4 (1%)	9	11
1	C	293/296 (99%)	281 (96%)	11 (4%)	1 (0%)	36	45
2	B	102/104 (98%)	90 (88%)	10 (10%)	2 (2%)	6	6
All	All	687/696 (99%)	648 (94%)	32 (5%)	7 (1%)	12	17

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%)	224 (89%)	28 (11%)	6	6
1	C	253/254 (100%)	225 (89%)	28 (11%)	6	6
2	B	86/86 (100%)	63 (73%)	23 (27%)	0	0
All	All	591/594 (100%)	512 (87%)	79 (13%)	4	3

All (79) 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	22	VAL
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	168	VAL
1	A	182	LEU
1	A	183	LYS
1	A	195	ASN
1	A	196	ASN
1	A	215	LYS
1	A	231	MET
1	A	267	GLU
1	A	269	LEU

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Mol	Chain	Res	Type
1	A	275	THR
1	A	289	LEU
2	B	4	GLU
2	B	8	LYS
2	B	11	VAL
2	B	12	GLN
2	B	19	THR
2	B	27	LYS
2	B	31	ASN
2	B	39	LYS
2	B	40	THR
2	B	61	GLU
2	B	64	LEU
2	B	65	MET
2	B	72	LYS
2	B	73	LYS
2	B	74	TYR
2	B	80	MET
2	B	81	ILE
2	B	91	ARG
2	B	94	LEU
2	B	98	LEU
2	B	99	LYS
2	B	103	ASN
2	B	104	GLU
1	C	0	ILE
1	C	28	LEU
1	C	32	GLU
1	C	53	ILE
1	C	63	THR
1	C	75	LYS
1	C	77	PHE
1	C	80	PRO
1	C	86	GLN
1	C	97	LYS
1	C	164	ASN
1	C	166	ARG
1	C	168	VAL
1	C	183	LYS
1	C	188	GLU
1	C	200	ASN
1	C	201	GLU

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Mol	Chain	Res	Type
1	C	207	LEU
1	C	210	ASP
1	C	219	ASN
1	C	226	LYS
1	C	230	MET
1	C	233	PRO
1	C	250	GLU
1	C	256	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 (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	38	ASN
1	A	86	GLN
1	A	96	HIS
1	A	195	ASN
1	A	196	ASN
1	A	220	ASN
1	A	222	GLN
1	A	255	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
1	C	222	GLN
1	C	292	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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	$\# Z > 2$
3	PO4	C	2202	-	4,4,4	2.57	1 (25%)	6,6,6	1.44	2 (33%)
4	ZNH	C	1201	1	50,50,50	1.08	4 (8%)	65,82,82	1.44	11 (16%)
3	PO4	A	2201	4,1	4,4,4	3.89	1 (25%)	6,6,6	1.86	2 (33%)
4	ZNH	A	1001	3,1	50,50,50	1.33	6 (12%)	65,82,82	1.62	15 (23%)
5	HEC	B	1101	2	50,50,50	1.89	16 (32%)	68,82,82	2.02	15 (22%)

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
4	ZNH	C	1201	1	1/1/3/9	4/14/54/54	-
4	ZNH	A	1001	3,1	1/1/3/9	3/14/54/54	-
5	HEC	B	1101	2	1/1/3/7	8/14/54/54	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2201	PO4	P-O1	7.52	1.68	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2202	PO4	P-O2	4.61	1.68	1.54
5	B	1101	HEC	CAB-C3B	-4.55	1.39	1.51
5	B	1101	HEC	FE-ND	3.67	2.06	1.94
5	B	1101	HEC	FE-NB	3.57	2.05	1.94
4	A	1001	ZNH	C3C-C4C	3.48	1.52	1.42
5	B	1101	HEC	CBB-CAB	-3.30	1.37	1.51
5	B	1101	HEC	C1A-NA	-3.25	1.33	1.39
5	B	1101	HEC	CHA-C4D	-2.96	1.32	1.39
5	B	1101	HEC	C4D-ND	-2.94	1.33	1.38
4	A	1001	ZNH	ZN-ND	2.84	2.12	2.03
4	A	1001	ZNH	CAC-C3C	-2.76	1.40	1.47
5	B	1101	HEC	CAC-C3C	-2.67	1.44	1.51
5	B	1101	HEC	C1D-C2D	2.63	1.49	1.44
5	B	1101	HEC	FE-NA	2.61	2.03	1.95
5	B	1101	HEC	C1D-ND	-2.58	1.35	1.40
4	C	1201	ZNH	ZN-NA	2.41	2.11	2.03
4	A	1001	ZNH	CMB-C2B	2.41	1.55	1.50
4	A	1001	ZNH	CAB-C3B	-2.41	1.41	1.47
4	C	1201	ZNH	CAC-C3C	-2.39	1.41	1.47
5	B	1101	HEC	FE-NC	2.34	2.02	1.95
4	C	1201	ZNH	CAB-C3B	-2.31	1.41	1.47
4	A	1001	ZNH	ZN-NC	2.20	2.10	2.03
4	C	1201	ZNH	C4D-C3D	2.14	1.48	1.45
5	B	1101	HEC	C4A-NA	-2.07	1.35	1.39
5	B	1101	HEC	CBC-CAC	-2.06	1.42	1.51
5	B	1101	HEC	CMD-C2D	2.04	1.54	1.50
5	B	1101	HEC	CHC-C4B	2.04	1.42	1.38

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1101	HEC	CBC-CAC-C3C	6.64	130.42	112.42
5	B	1101	HEC	CBB-CAB-C3B	5.71	127.90	112.42
5	B	1101	HEC	C3D-C4D-ND	4.73	114.92	110.35
5	B	1101	HEC	CMD-C2D-C1D	4.36	131.84	125.03
5	B	1101	HEC	C1A-CHA-C4D	3.97	134.45	126.02
5	B	1101	HEC	C1D-C2D-C3D	-3.63	103.16	106.98
4	A	1001	ZNH	C2C-C1C-NC	3.60	113.54	109.02
5	B	1101	HEC	CAB-C3B-C4B	3.47	129.31	124.79
5	B	1101	HEC	CHD-C1D-ND	-3.41	120.15	124.37
5	B	1101	HEC	CHC-C4B-C3B	3.34	131.39	125.23
4	A	1001	ZNH	C4C-C3C-C2C	-3.32	103.17	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1201	ZNH	CBA-CAA-C2A	3.28	121.61	112.53
5	B	1101	HEC	C2D-C1D-ND	2.97	113.25	109.84
4	A	1001	ZNH	C1A-CHA-C4D	2.93	132.24	126.02
4	C	1201	ZNH	CHC-C4B-NB	-2.90	121.00	124.75
4	A	1001	ZNH	CAA-C2A-C3A	2.89	133.28	127.87
4	A	1001	ZNH	C2D-C1D-ND	2.78	112.64	109.06
5	B	1101	HEC	C2A-C1A-NA	2.73	112.96	110.32
4	C	1201	ZNH	CHD-C1D-ND	-2.73	121.22	124.75
3	A	2201	PO4	O3-P-O1	-2.73	101.29	110.95
5	B	1101	HEC	CHC-C4B-NB	-2.72	121.00	124.37
5	B	1101	HEC	CAB-C3B-C2B	-2.71	122.57	127.56
5	B	1101	HEC	CHA-C4D-ND	-2.65	121.57	124.42
4	A	1001	ZNH	CHD-C1D-ND	-2.65	121.33	124.75
4	C	1201	ZNH	CMA-C3A-C4A	2.63	129.36	124.73
4	A	1001	ZNH	CMC-C2C-C1C	-2.56	121.52	125.42
3	A	2201	PO4	O4-P-O3	2.52	115.75	107.91
3	C	2202	PO4	O4-P-O3	2.52	115.75	107.91
4	A	1001	ZNH	CBA-CAA-C2A	2.52	119.49	112.53
4	A	1001	ZNH	C1D-ND-C4D	-2.51	103.14	106.47
4	C	1201	ZNH	C4A-NA-C1A	-2.44	102.89	106.52
4	C	1201	ZNH	C4A-C3A-C2A	-2.43	103.37	106.97
5	B	1101	HEC	C3B-C4B-NB	-2.34	107.61	110.17
4	A	1001	ZNH	CHB-C4A-NA	-2.34	120.95	124.82
4	C	1201	ZNH	CMB-C2B-C1B	-2.30	121.44	125.03
4	C	1201	ZNH	CHA-C4D-ND	-2.30	120.75	124.77
4	C	1201	ZNH	C2D-C1D-ND	2.29	112.01	109.06
4	A	1001	ZNH	CHC-C4B-NB	-2.24	121.86	124.75
4	A	1001	ZNH	C4B-C3B-C2B	-2.21	105.25	107.28
4	C	1201	ZNH	C3A-C4A-NA	2.18	113.68	110.35
4	A	1001	ZNH	C3D-C4D-ND	2.16	114.20	110.16
4	A	1001	ZNH	C1C-CHC-C4B	2.16	131.32	126.25
3	C	2202	PO4	O3-P-O2	-2.12	101.30	107.91
4	A	1001	ZNH	CHA-C4D-ND	-2.09	121.11	124.77
4	C	1201	ZNH	C1A-CHA-C4D	2.06	130.40	126.02

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1001	ZNH	NA
4	C	1201	ZNH	NA
5	B	1101	HEC	NA

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1101	HEC	C2C-C3C-CAC-CBC
5	B	1101	HEC	C4C-C3C-CAC-CBC
5	B	1101	HEC	C3A-C2A-CAA-CBA
5	B	1101	HEC	C2A-CAA-CBA-CGA
5	B	1101	HEC	CAA-CBA-CGA-O1A
4	A	1001	ZNH	CAA-CBA-CGA-O2A
4	C	1201	ZNH	CAA-CBA-CGA-O2A
4	C	1201	ZNH	CAA-CBA-CGA-O1A
4	A	1001	ZNH	CAA-CBA-CGA-O1A
5	B	1101	HEC	CAA-CBA-CGA-O2A
4	C	1201	ZNH	CAD-CBD-CGD-O2D
4	C	1201	ZNH	CAD-CBD-CGD-O1D
5	B	1101	HEC	CAD-CBD-CGD-O2D
5	B	1101	HEC	CAD-CBD-CGD-O1D
4	A	1001	ZNH	CAD-CBD-CGD-O2D

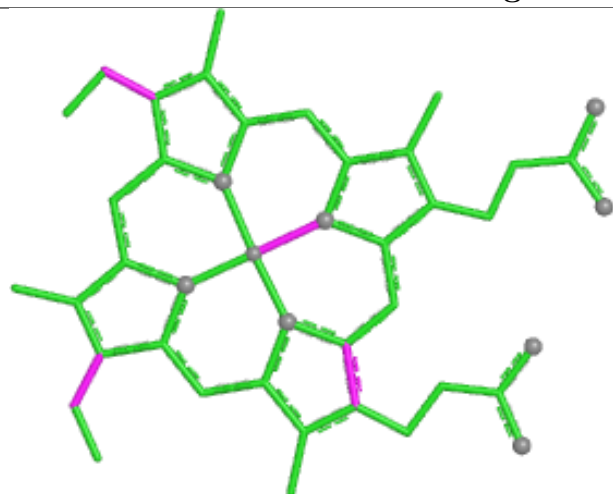
There are no ring outliers.

5 monomers are involved in 21 short contacts:

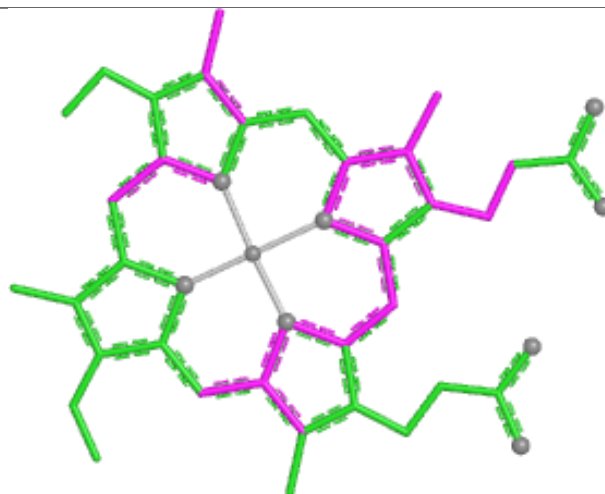
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2202	PO4	9	0
4	C	1201	ZNH	5	0
3	A	2201	PO4	2	0
4	A	1001	ZNH	6	0
5	B	1101	HEC	4	0

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

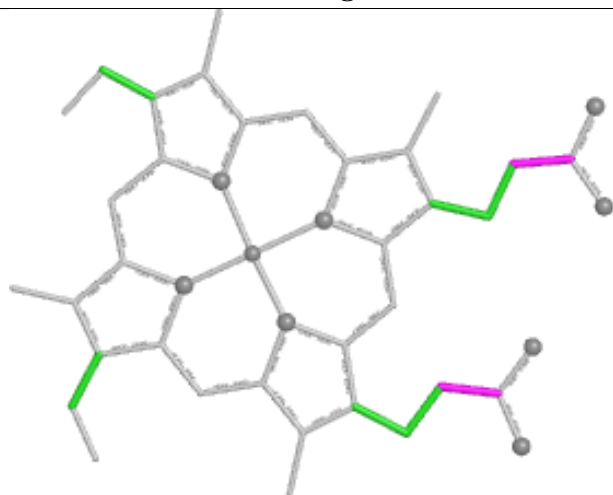
Ligand ZNH C 1201



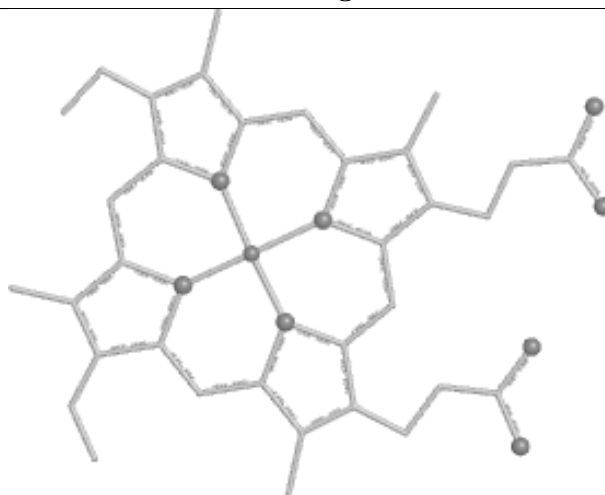
Bond lengths



Bond angles

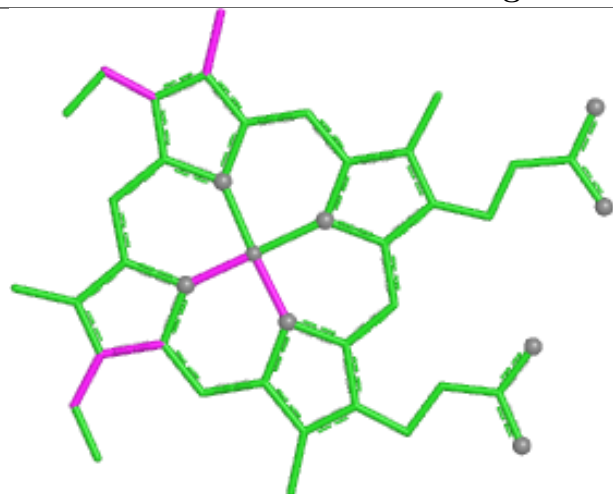


Torsions

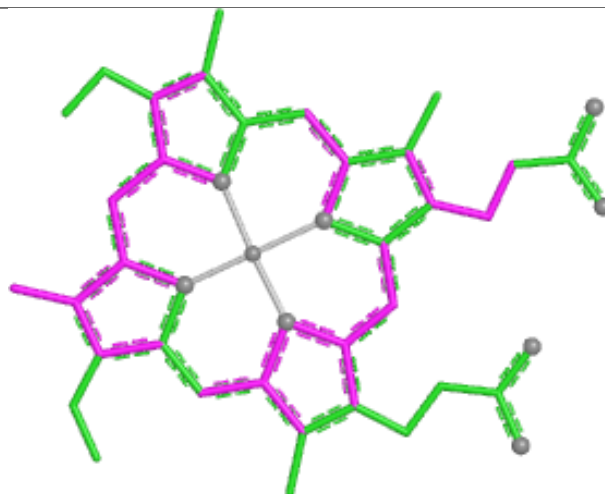


Rings

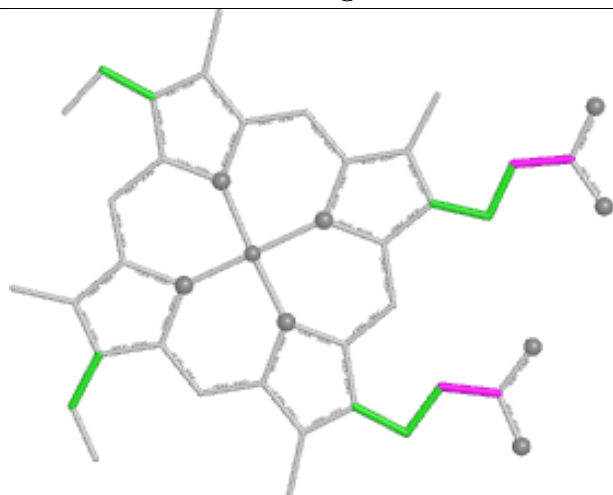
Ligand ZNH A 1001



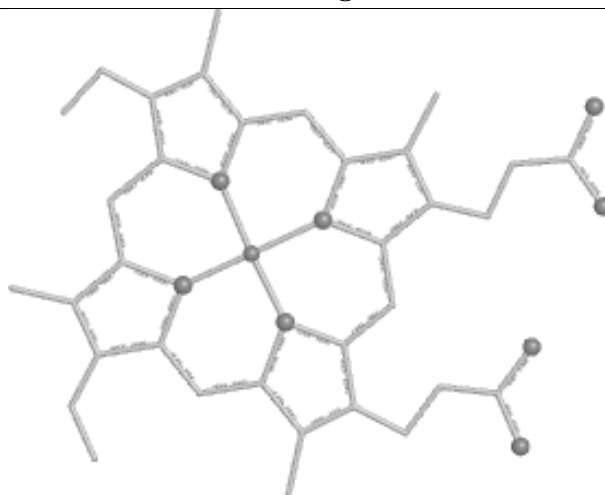
Bond lengths



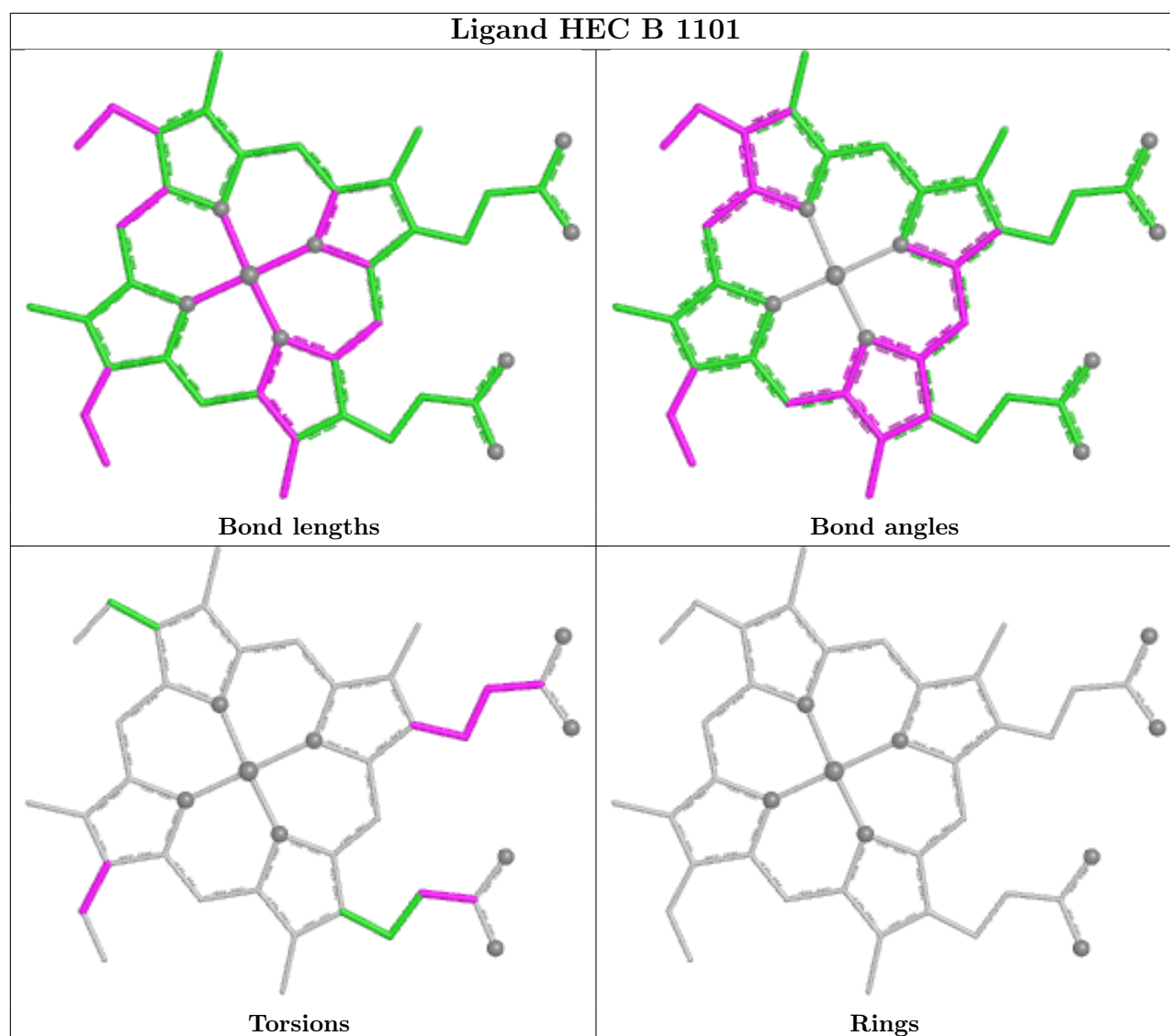
Bond angles



Torsions



Rings



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%)	0.46	7 (2%) 59 61	46, 56, 69, 101	0
1	C	295/296 (99%)	0.42	6 (2%) 65 65	45, 57, 67, 87	0
2	B	104/104 (100%)	2.63	70 (67%) 0 0	40, 62, 72, 75	0
All	All	693/696 (99%)	0.77	83 (11%) 9 8	40, 57, 70, 101	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	3	VAL	5.9
2	B	1	GLY	5.5
2	B	51	ALA	5.3
2	B	4	GLU	5.1
2	B	83	ALA	5.1
2	B	36	PHE	5.0
2	B	12	GLN	4.9
2	B	80	MET	4.7
2	B	68	LEU	4.5
2	B	29	GLY	4.4
1	A	3	PRO	4.3
2	B	59	TRP	4.2
2	B	9	ILE	4.2
2	B	11	VAL	4.1
2	B	30	PRO	4.0
2	B	57	ILE	3.9
2	B	96	ALA	3.9
2	B	35	LEU	3.9
2	B	66	GLU	3.8
2	B	102	THR	3.6
2	B	62	GLU	3.6
2	B	74	TYR	3.6
2	B	101	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	2	ASP	3.4
2	B	13	LYS	3.4
2	B	98	LEU	3.3
2	B	73	LYS	3.3
2	B	100	LYS	3.2
2	B	67	TYR	3.2
2	B	47	THR	3.2
2	B	90	GLU	3.2
2	B	31	ASN	3.2
2	B	87	LYS	3.2
1	A	2	THR	3.2
2	B	58	THR	3.2
2	B	43	ALA	3.1
2	B	8	LYS	3.1
2	B	97	TYR	3.1
2	B	81	ILE	3.1
2	B	19	THR	3.0
2	B	15	ALA	3.0
1	A	137	THR	2.9
2	B	25	LYS	2.9
1	C	77	PHE	2.9
2	B	94	LEU	2.8
2	B	82	PHE	2.8
2	B	71	PRO	2.8
2	B	5	LYS	2.7
1	C	257	LYS	2.7
1	A	1	THR	2.7
2	B	6	GLY	2.7
2	B	32	LEU	2.7
1	A	22	VAL	2.6
1	C	237	SER	2.6
2	B	70	ASN	2.6
2	B	14	CYS	2.6
2	B	93	ASP	2.5
2	B	95	ILE	2.5
2	B	52	ASN	2.5
1	A	279	ASP	2.5
2	B	104	GLU	2.4
2	B	56	GLY	2.4
2	B	34	GLY	2.4
2	B	33	HIS	2.4
2	B	69	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	77	GLY	2.3
2	B	46	PHE	2.3
2	B	45	GLY	2.3
1	A	10	VAL	2.3
2	B	85	ILE	2.2
2	B	21	GLU	2.2
1	C	194	ALA	2.2
1	C	260	LYS	2.2
2	B	16	GLN	2.1
2	B	99	LYS	2.1
2	B	10	PHE	2.1
2	B	49	THR	2.1
2	B	23	GLY	2.1
2	B	39	LYS	2.1
2	B	18	HIS	2.1
2	B	54	ASN	2.0
1	C	215	LYS	2.0
2	B	28	THR	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](#)

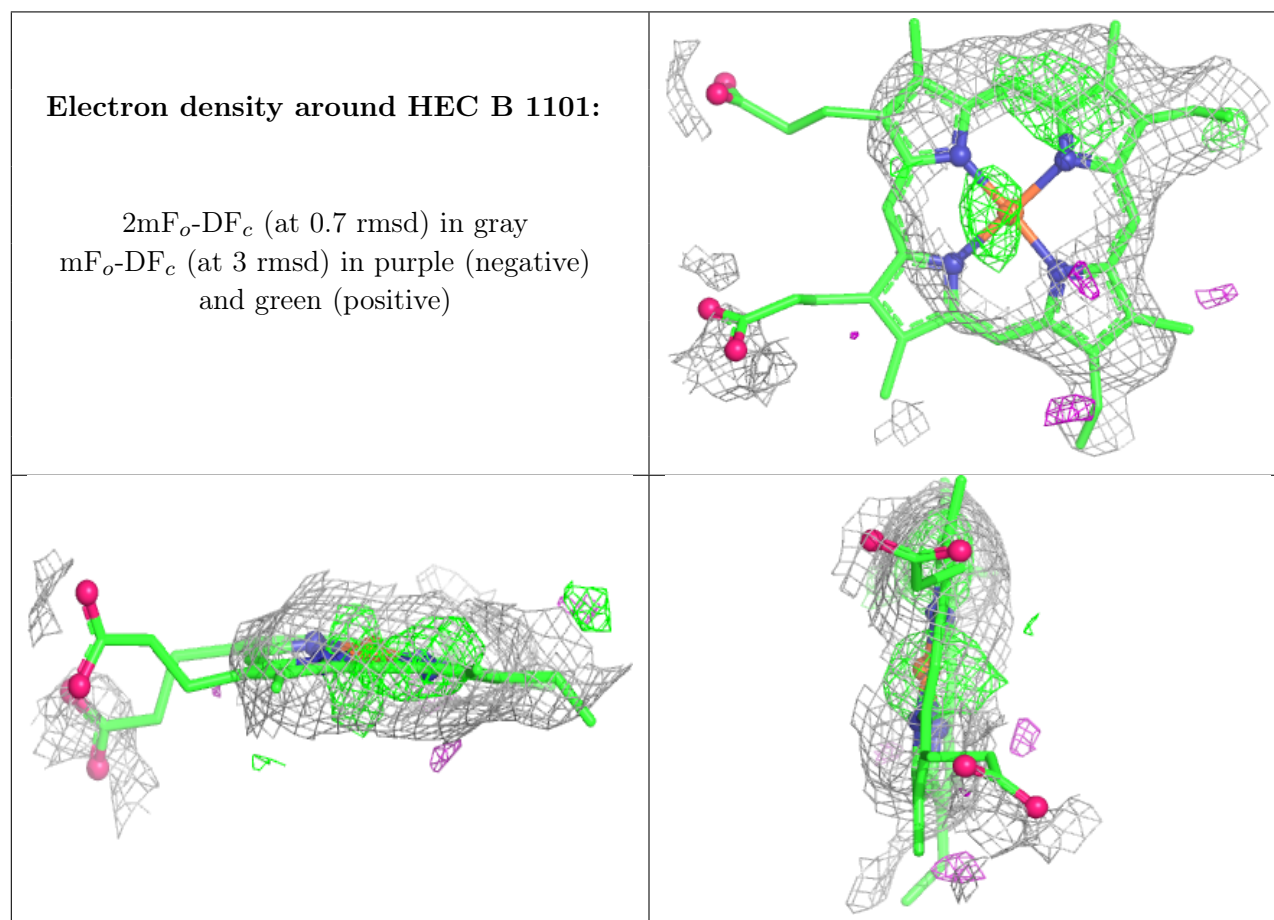
There are no oligosaccharides in this entry.

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.

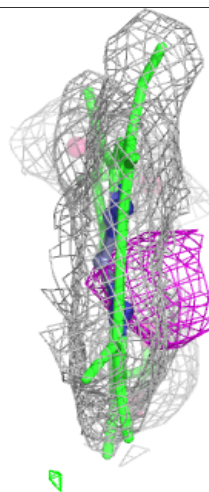
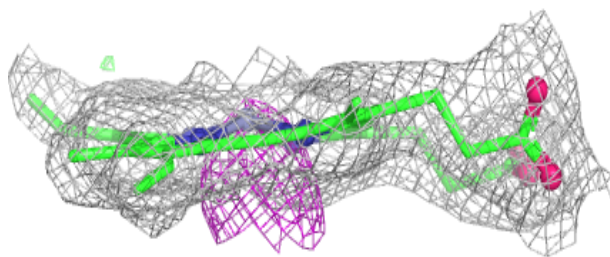
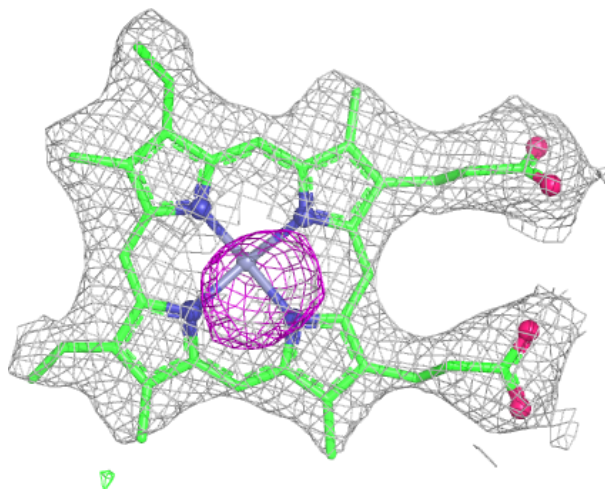
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	A	2201	5/5	0.71	0.48	83,96,99,105	0
3	PO4	C	2202	5/5	0.76	0.46	98,106,106,114	0
5	HEC	B	1101	43/43	0.89	0.19	45,51,59,65	0
4	ZNH	C	1201	43/43	0.96	0.10	47,56,60,61	0
4	ZNH	A	1001	43/43	0.96	0.10	46,54,57,65	0

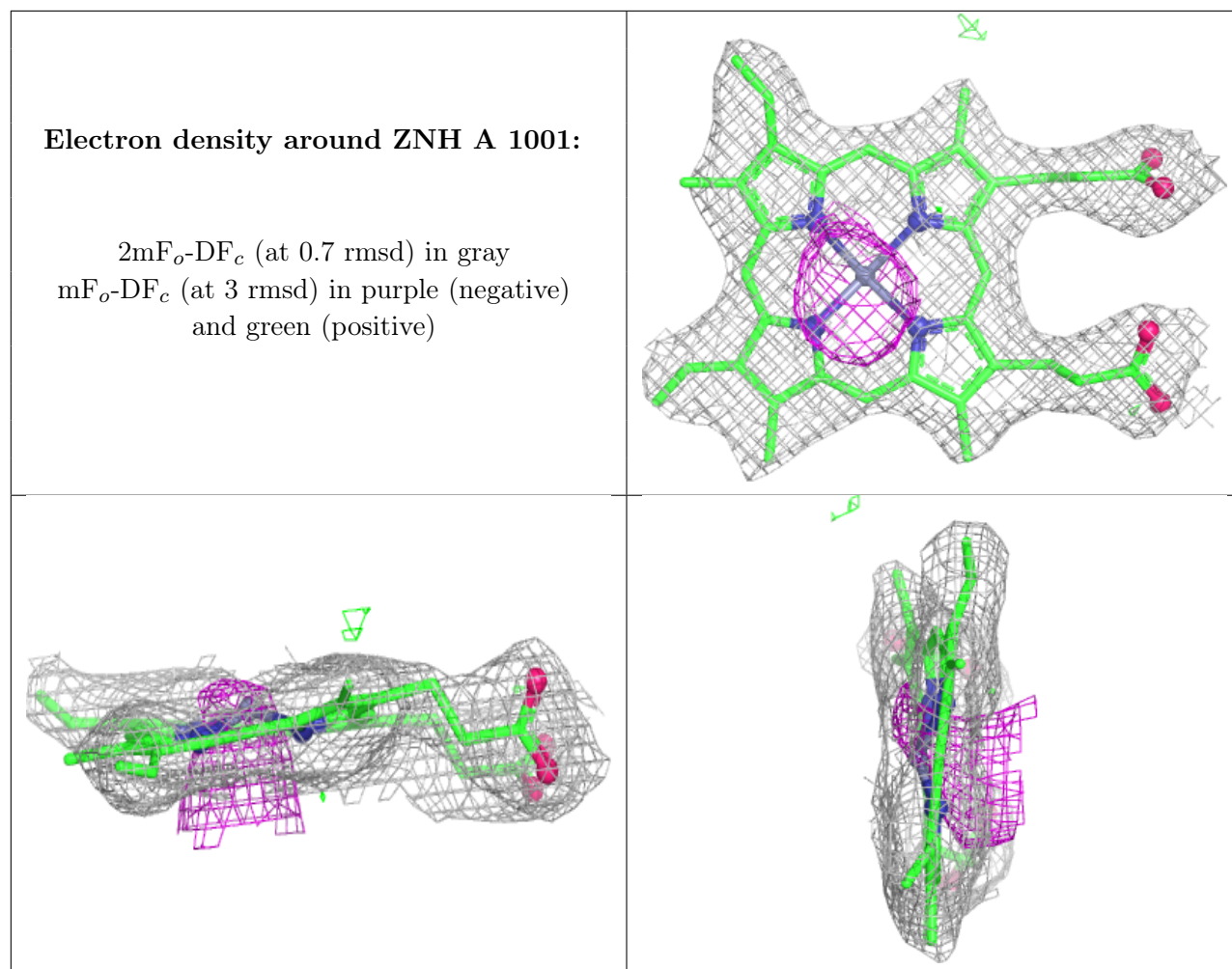
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around 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.