



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:07 PM UTC

PDB ID : 4B2N / pdb_00004b2n
Title : Latex Oxygenase RoxA
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Deposited on : 2012-07-17
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

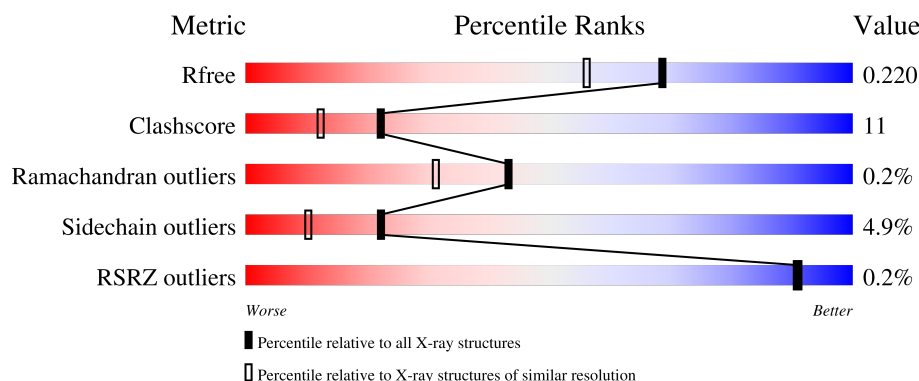
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	662	 79% 17% ..
1	B	662	 77% 18% ..

2 Entry composition (i)

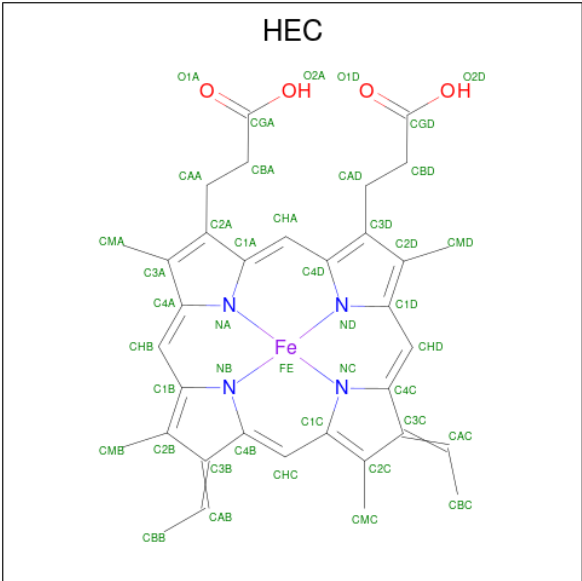
There are 5 unique types of molecules in this entry. The entry contains 12168 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 70 KDA PROTEIN.

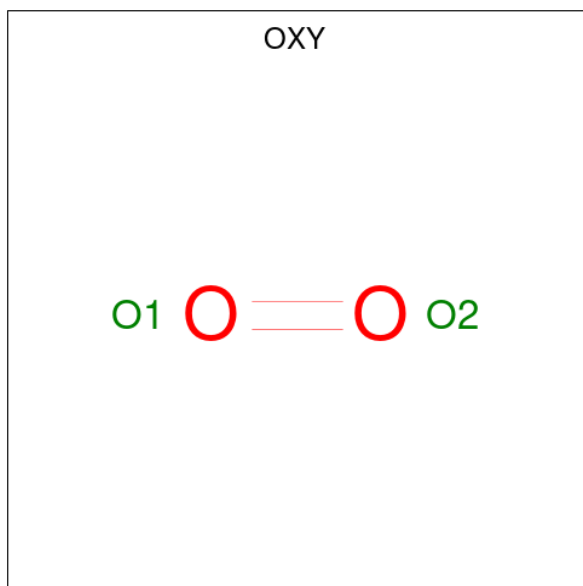
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	648	Total	C	N	O	S	0	4	0
			5096	3246	891	940	19			
1	B	648	Total	C	N	O	S	0	5	0
			5104	3251	892	941	20			

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



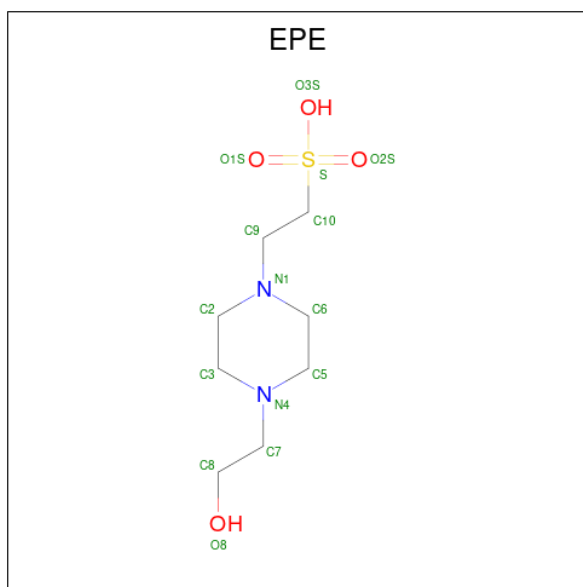
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



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

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

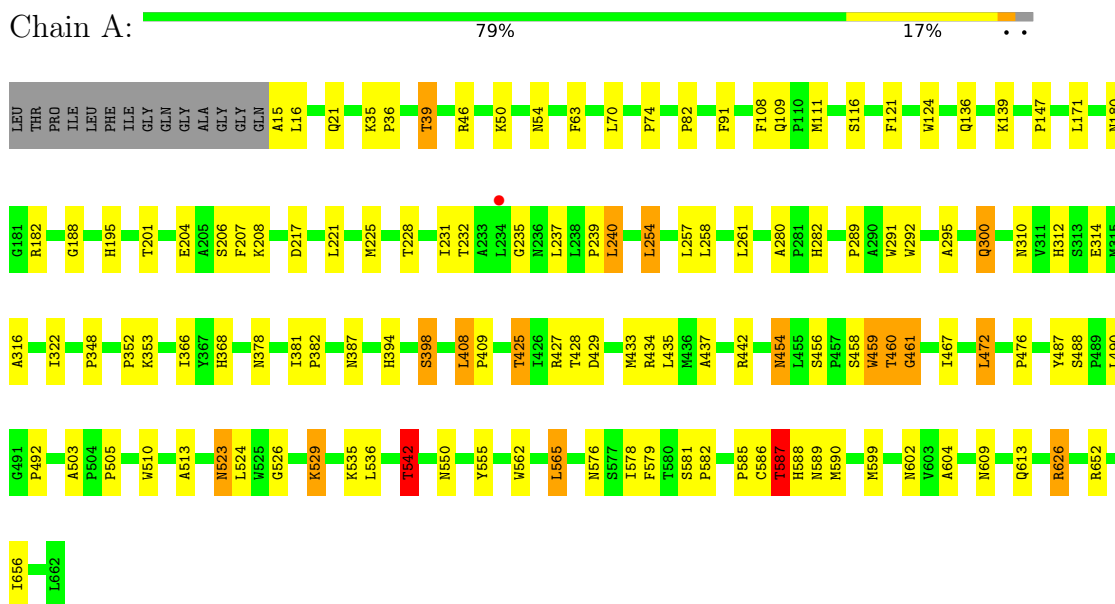
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	907	Total	O	0	0
			907	907		
5	B	855	Total	O	0	0
			855	855		

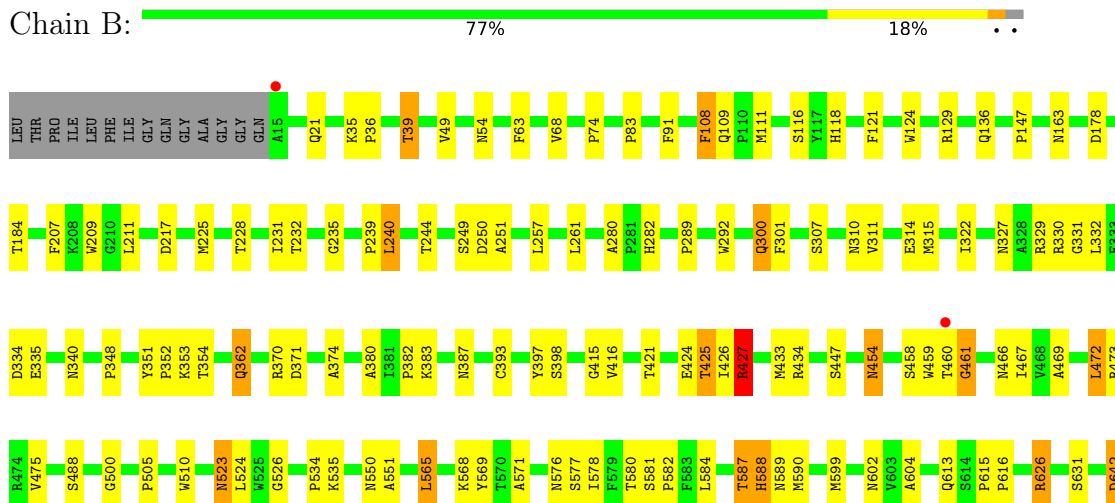
3 Residue-property plots

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

• Molecule 1: 70 KDA PROTEIN



• Molecule 1: 70 KDA PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.37Å 97.11Å 101.05Å 90.00° 98.39° 90.00°	Depositor
Resolution (Å)	35.80 – 1.80 35.80 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (35.80-1.80) 69.6 (35.80-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.168 , 0.220 0.168 , 0.220	Depositor DCC
R_{free} test set	6420 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12168	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: HEC, EPE, OXY

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	1.29	15/5261 (0.3%)	1.25	27/7198 (0.4%)
1	B	1.23	10/5269 (0.2%)	1.23	25/7208 (0.3%)
All	All	1.26	25/10530 (0.2%)	1.24	52/14406 (0.4%)

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
1	A	0	1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	PRO	CA-C	9.21	1.56	1.51
1	B	209	TRP	C-O	6.58	1.31	1.23
1	B	249	SER	C-O	6.47	1.31	1.23
1	A	513	ALA	CA-C	6.25	1.60	1.53
1	A	195	HIS	ND1-CE1	5.98	1.38	1.32
1	A	588	HIS	CG-CD2	5.95	1.42	1.35
1	A	21	GLN	C-O	-5.84	1.16	1.24
1	B	91	PHE	C-O	5.78	1.30	1.24
1	A	588	HIS	CE1-NE2	5.71	1.38	1.32
1	A	195	HIS	CE1-NE2	5.65	1.38	1.32
1	A	505	PRO	C-O	5.61	1.30	1.23
1	A	282	HIS	CG-CD2	5.51	1.42	1.35
1	B	282	HIS	CG-CD2	5.51	1.42	1.35
1	B	626	ARG	CD-NE	-5.46	1.38	1.46
1	A	555	TYR	N-CA	5.38	1.52	1.46
1	A	82	PRO	CA-C	5.22	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	459	TRP	CA-C	-5.17	1.45	1.52
1	B	505	PRO	C-O	5.14	1.29	1.23
1	A	312	HIS	ND1-CE1	5.12	1.37	1.32
1	B	330	ARG	C-O	-5.12	1.17	1.24
1	A	91	PHE	C-O	5.08	1.30	1.24
1	B	588	HIS	CG-CD2	5.05	1.41	1.35
1	B	473	ARG	C-O	-5.04	1.17	1.24
1	A	291	TRP	CD2-CE2	5.03	1.50	1.41
1	A	626	ARG	CD-NE	-5.03	1.39	1.46

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	626	ARG	NE-CZ-NH2	-10.96	109.33	119.20
1	A	626	ARG	NE-CZ-NH2	-10.67	109.59	119.20
1	A	488	SER	CA-C-N	-8.50	111.62	120.03
1	A	488	SER	C-N-CA	-8.50	111.62	120.03
1	A	542	THR	N-CA-CB	-8.49	98.75	110.38
1	A	587	THR	CB-CA-C	-7.64	93.88	109.38
1	B	447	SER	CA-C-N	-7.52	112.88	121.83
1	B	447	SER	C-N-CA	-7.52	112.88	121.83
1	A	626	ARG	CG-CD-NE	-7.30	95.93	112.00
1	B	568	LYS	N-CA-C	-7.11	100.47	110.50
1	B	626	ARG	CG-CD-NE	-6.78	97.08	112.00
1	A	231	ILE	N-CA-C	-6.63	104.02	110.72
1	B	74	PRO	CB-CA-C	-6.61	105.17	111.39
1	A	235	GLY	N-CA-C	6.46	119.43	112.33
1	B	616	PRO	CA-C-N	-6.42	111.03	120.46
1	B	616	PRO	C-N-CA	-6.42	111.03	120.46
1	B	626	ARG	NE-CZ-NH1	6.34	127.84	121.50
1	A	503	ALA	CA-C-N	-6.10	114.10	120.38
1	A	503	ALA	C-N-CA	-6.10	114.10	120.38
1	B	488	SER	CA-C-N	-6.08	113.71	119.85
1	B	488	SER	C-N-CA	-6.08	113.71	119.85
1	A	435	LEU	CA-C-N	-6.07	113.00	123.25
1	A	435	LEU	C-N-CA	-6.07	113.00	123.25
1	A	171	LEU	CA-C-N	-5.77	115.29	123.08
1	A	171	LEU	C-N-CA	-5.77	115.29	123.08
1	B	615	PRO	CA-C-N	-5.76	115.51	119.66
1	B	615	PRO	C-N-CA	-5.76	115.51	119.66
1	B	475	VAL	CA-C-N	-5.66	113.84	119.56
1	B	475	VAL	C-N-CA	-5.66	113.84	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	280	ALA	CA-C-N	-5.62	114.17	119.85
1	B	280	ALA	C-N-CA	-5.62	114.17	119.85
1	A	258	LEU	CA-C-N	-5.59	114.06	119.87
1	A	258	LEU	C-N-CA	-5.59	114.06	119.87
1	A	433	MET	CB-CG-SD	-5.58	95.97	112.70
1	B	584	LEU	CA-C-N	5.55	125.54	120.21
1	B	584	LEU	C-N-CA	5.55	125.54	120.21
1	B	626	ARG	CD-NE-CZ	5.47	132.06	124.40
1	A	74	PRO	CA-C-N	-5.40	114.82	120.38
1	A	74	PRO	C-N-CA	-5.40	114.82	120.38
1	A	467	ILE	N-CA-C	-5.39	105.27	110.72
1	B	329	ARG	N-CA-C	-5.31	105.41	111.14
1	B	231	ILE	N-CA-C	-5.20	105.64	110.53
1	B	433	MET	CB-CG-SD	-5.19	97.12	112.70
1	A	366	ILE	N-CA-C	-5.17	105.46	110.42
1	A	456	SER	CA-C-N	-5.17	114.34	119.56
1	A	456	SER	C-N-CA	-5.17	114.34	119.56
1	B	427	ARG	N-CA-C	5.05	118.57	111.90
1	B	551	ALA	N-CA-C	-5.04	103.49	110.35
1	A	378	ASN	CA-C-N	5.02	125.65	120.03
1	A	378	ASN	C-N-CA	5.02	125.65	120.03
1	A	280	ALA	CA-C-N	-5.01	114.79	119.85
1	A	280	ALA	C-N-CA	-5.01	114.79	119.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	459	TRP	Peptide

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	5096	0	4894	106	0
1	B	5104	0	4903	110	0
2	A	86	0	60	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	86	0	61	7	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	15	0	18	1	0
4	B	15	0	18	0	0
5	A	907	0	0	21	0
5	B	855	0	0	21	0
All	All	12168	0	9954	215	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 11.

All (215) 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:B:393:CYS:SG	2:B:701:HEC:CAC	2.09	1.40
1:B:393:CYS:SG	2:B:701:HEC:HAC	1.78	1.11
1:A:240[A]:LEU:HD21	1:A:599:MET:HE3	1.19	1.09
1:B:240[A]:LEU:HD21	1:B:599[A]:MET:HE3	1.30	1.05
1:B:645:GLN:HG3	5:B:2837:HOH:O	1.58	1.01
1:B:427:ARG:HG3	1:B:427:ARG:HH11	1.23	0.98
1:B:163:ASN:HB3	5:B:2309:HOH:O	1.65	0.95
1:A:35:LYS:HB3	1:A:39:THR:HG21	1.48	0.93
1:A:111:MET:HG2	1:A:240[B]:LEU:CD1	2.02	0.90
1:B:36:PRO:O	1:B:39:THR:HG23	1.73	0.89
1:A:460:THR:HB	5:A:2719:HOH:O	1.72	0.89
1:B:35:LYS:HB3	1:B:39:THR:HG21	1.58	0.85
1:B:232:THR:HG23	1:B:235:GLY:HA3	1.58	0.84
1:B:240[A]:LEU:HD23	1:B:599[A]:MET:HG2	1.59	0.82
1:B:108:PHE:CZ	1:B:240[B]:LEU:HD22	2.14	0.82
1:B:240[A]:LEU:CD2	1:B:599[A]:MET:HG2	2.10	0.81
1:A:239:PRO:O	1:A:240[B]:LEU:HD23	1.81	0.81
1:B:111:MET:HE3	1:B:225:MET:HE3	1.63	0.80
1:B:240[A]:LEU:HD21	1:B:599[A]:MET:CE	2.10	0.80
1:B:602:ASN:ND2	1:B:613:GLN:H	1.81	0.79
1:A:36:PRO:O	1:A:39:THR:HG23	1.82	0.79
1:B:240[A]:LEU:HD23	1:B:240[A]:LEU:O	1.83	0.79
1:A:180:ASN:HD22	1:B:571:ALA:H	1.29	0.79
1:B:111:MET:HG2	1:B:240[B]:LEU:CD1	2.13	0.78
1:A:108:PHE:CZ	1:A:240[B]:LEU:HD22	2.18	0.78
1:A:240[A]:LEU:HD23	1:A:599:MET:HG2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:THR:CG2	1:B:235:GLY:HA3	2.14	0.77
1:A:576:ASN:ND2	1:A:586:CYS:H	1.83	0.76
1:B:118:HIS:CD2	1:B:129:ARG:NH2	2.53	0.76
1:A:109:GLN:HB3	1:A:240[B]:LEU:HD21	1.68	0.75
1:B:588:HIS:HB3	5:B:2791:HOH:O	1.85	0.74
1:B:334[B]:ASP:OD1	1:B:335:GLU:N	2.21	0.73
1:A:609:ASN:OD1	5:A:2856:HOH:O	2.06	0.73
1:A:201:THR:OG1	1:A:204:GLU:HG3	1.90	0.72
1:A:240[A]:LEU:HD21	1:A:599:MET:CE	2.11	0.72
1:A:111:MET:HE3	1:A:225:MET:HE3	1.71	0.72
1:B:427:ARG:HG3	1:B:427:ARG:NH1	2.00	0.72
1:A:565:LEU:HD22	1:A:656:ILE:HG23	1.71	0.71
1:B:118:HIS:CD2	1:B:129:ARG:HH22	2.08	0.71
1:B:393:CYS:SG	2:B:701:HEC:C3C	2.79	0.71
1:A:576:ASN:HD21	1:A:586:CYS:H	1.36	0.71
1:A:454:ASN:HD22	1:A:454:ASN:H	1.39	0.70
1:B:21:GLN:HG2	5:B:2287:HOH:O	1.90	0.70
1:A:217:ASP:OD2	1:A:626:ARG:HD3	1.93	0.69
1:B:54:ASN:HD21	1:B:63:PHE:H	1.40	0.69
1:B:35:LYS:HE3	5:B:2046:HOH:O	1.92	0.67
1:A:54:ASN:HD21	1:A:63:PHE:H	1.42	0.67
1:A:460:THR:O	1:A:461:GLY:O	2.12	0.67
1:A:139:LYS:HE2	1:A:542:THR:CG2	2.24	0.67
1:A:427:ARG:HD3	5:A:2680:HOH:O	1.94	0.67
1:B:240[A]:LEU:HD23	1:B:240[A]:LEU:H	1.59	0.67
1:A:139:LYS:HE2	1:A:542:THR:HG21	1.75	0.66
1:A:490:LEU:HD13	5:A:2391:HOH:O	1.95	0.66
1:A:602:ASN:ND2	1:A:613:GLN:H	1.93	0.66
1:A:136:GLN:HE21	1:A:550:ASN:HD22	1.43	0.66
1:B:240[B]:LEU:HD23	5:B:2467:HOH:O	1.96	0.65
1:A:180:ASN:ND2	1:B:571:ALA:H	1.94	0.65
1:A:240[A]:LEU:CD2	1:A:599:MET:HG2	2.27	0.65
1:B:371:ASP:HB3	1:B:374:ALA:HB2	1.79	0.65
1:B:424:GLU:HB2	5:B:2652:HOH:O	1.97	0.64
1:B:460:THR:O	1:B:461:GLY:O	2.15	0.64
1:B:523:ASN:ND2	1:B:526:GLY:H	1.97	0.63
1:B:147:PRO:HG3	1:B:207:PHE:CD2	2.34	0.63
1:A:458:SER:HB3	5:A:2715:HOH:O	1.98	0.63
1:A:111:MET:CG	1:A:240[B]:LEU:CD1	2.77	0.62
1:A:458:SER:CB	5:A:2715:HOH:O	2.46	0.62
1:B:217:ASP:OD2	1:B:626:ARG:HD3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240[A]:LEU:HD23	1:B:240[A]:LEU:N	2.15	0.62
1:A:36:PRO:O	1:A:39:THR:CG2	2.49	0.60
1:B:240[A]:LEU:HD23	1:B:240[A]:LEU:C	2.25	0.60
1:A:111:MET:SD	1:A:240[B]:LEU:HD13	2.41	0.60
1:A:136:GLN:NE2	1:A:550:ASN:HD22	2.00	0.60
1:A:472:LEU:C	1:A:472:LEU:HD23	2.27	0.60
1:A:15:ALA:HB1	5:A:2004:HOH:O	2.02	0.59
1:B:111:MET:SD	1:B:240[B]:LEU:HD13	2.41	0.59
1:B:240[A]:LEU:CD2	1:B:240[A]:LEU:N	2.65	0.59
1:B:454:ASN:H	1:B:454:ASN:HD22	1.50	0.59
1:A:111:MET:HG2	1:A:240[B]:LEU:HD11	1.85	0.59
1:A:182[B]:ARG:HD2	5:A:2370:HOH:O	2.02	0.59
1:A:15:ALA:HB3	5:A:2003:HOH:O	2.01	0.59
1:B:111:MET:CE	1:B:225:MET:HE3	2.32	0.58
1:B:393:CYS:SG	2:B:701:HEC:CBC	2.89	0.58
1:B:240[A]:LEU:CD2	1:B:599[A]:MET:HE3	2.20	0.57
1:B:111:MET:CG	1:B:240[B]:LEU:CD1	2.82	0.57
1:A:523:ASN:HD22	1:A:523:ASN:C	2.12	0.56
1:B:239:PRO:O	1:B:240[B]:LEU:HD23	2.05	0.56
1:B:244:THR:HG21	5:B:2832:HOH:O	2.05	0.56
1:B:353:LYS:NZ	5:B:2582:HOH:O	2.39	0.56
1:A:536:LEU:N	1:A:536:LEU:HD12	2.21	0.56
1:A:579:PHE:HB3	5:A:2829:HOH:O	2.06	0.56
1:A:602:ASN:HD22	1:A:613:GLN:H	1.53	0.56
1:B:425:THR:HG21	5:B:2347:HOH:O	2.04	0.56
1:A:36:PRO:HG2	1:A:39:THR:HG22	1.89	0.55
1:B:109:GLN:HB3	1:B:240[B]:LEU:HD21	1.88	0.55
1:B:108:PHE:CE1	1:B:240[B]:LEU:HD22	2.42	0.55
1:B:136:GLN:HE21	1:B:550:ASN:HD22	1.55	0.55
1:A:240[A]:LEU:HD23	1:A:240[A]:LEU:N	2.21	0.55
1:B:232:THR:HG23	1:B:235:GLY:CA	2.33	0.55
1:A:108:PHE:CE1	1:A:240[B]:LEU:HD22	2.42	0.54
1:B:136:GLN:NE2	1:B:550:ASN:HD22	2.04	0.54
1:B:523:ASN:C	1:B:523:ASN:HD22	2.15	0.54
1:B:240[B]:LEU:CD2	5:B:2467:HOH:O	2.53	0.54
1:B:147:PRO:HG3	1:B:207:PHE:CG	2.42	0.54
1:B:383:LYS:HE2	5:B:2615:HOH:O	2.06	0.53
1:B:426:ILE:C	1:B:427:ARG:HG2	2.33	0.53
1:B:565:LEU:HD22	1:B:656:ILE:HG23	1.89	0.53
1:A:314:GLU:HG2	2:A:700:HEC:HMA2	1.89	0.53
1:B:454:ASN:ND2	5:B:2678:HOH:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:MET:HG2	1:A:240[B]:LEU:HD12	1.86	0.53
1:A:111:MET:HE3	1:A:225:MET:HG3	1.91	0.53
1:A:587:THR:HB	1:A:589:ASN:H	1.73	0.53
1:B:36:PRO:O	1:B:39:THR:CG2	2.53	0.53
1:A:460:THR:CB	5:A:2719:HOH:O	2.45	0.53
1:A:454:ASN:HD22	1:A:454:ASN:N	2.07	0.52
1:B:362:GLN:HG2	5:B:2593:HOH:O	2.10	0.52
1:B:461:GLY:HA2	5:B:2689:HOH:O	2.08	0.52
1:A:240[A]:LEU:HD23	1:A:240[A]:LEU:H	1.74	0.52
1:B:240[A]:LEU:CD2	1:B:240[A]:LEU:H	2.23	0.52
1:B:314:GLU:HG2	2:B:700:HEC:HMA2	1.92	0.52
1:B:311:VAL:O	1:B:315:MET:HG3	2.10	0.51
1:B:466:ASN:ND2	1:B:469:ALA:H	2.08	0.51
1:A:232:THR:HG23	5:A:2491:HOH:O	2.11	0.50
1:B:581:SER:HA	1:B:582:PRO:C	2.35	0.50
1:A:613:GLN:NE2	5:A:2864:HOH:O	2.44	0.50
1:B:39:THR:HB	5:B:2032:HOH:O	2.11	0.49
1:B:577:SER:HB2	1:B:580:THR:HG23	1.93	0.49
1:A:585:PRO:CB	1:A:590:MET:HB2	2.42	0.49
1:A:382:PRO:O	1:A:425:THR:HB	2.11	0.49
1:B:534:PRO:HG3	1:B:569:TYR:CE2	2.48	0.49
1:A:427:ARG:CD	5:A:2680:HOH:O	2.55	0.49
1:B:352:PRO:HD3	1:B:510:TRP:CH2	2.47	0.49
1:B:535:LYS:O	1:B:631:SER:HB2	2.12	0.49
1:A:394:HIS:CE1	2:A:701:HEC:NA	2.81	0.48
1:A:240[A]:LEU:CD2	1:A:240[A]:LEU:N	2.76	0.48
1:A:240[A]:LEU:HD23	1:A:240[A]:LEU:O	2.12	0.48
1:A:352:PRO:HD3	1:A:510:TRP:CH2	2.48	0.48
1:B:240[B]:LEU:HD23	1:B:240[B]:LEU:HA	1.47	0.48
1:B:472:LEU:HD23	1:B:472:LEU:C	2.39	0.48
1:B:315:MET:HE3	1:B:332:LEU:HB2	1.96	0.48
1:A:147:PRO:HG3	1:A:207:PHE:CD2	2.48	0.48
1:A:240[A]:LEU:HD23	1:A:240[A]:LEU:C	2.39	0.48
1:B:116:SER:HB3	1:B:228:THR:HB	1.96	0.47
1:A:454:ASN:ND2	5:A:2713:HOH:O	2.47	0.47
1:A:381:ILE:HG12	1:A:427:ARG:NH1	2.30	0.47
1:A:254:LEU:HD13	1:A:316:ALA:HB1	1.96	0.47
1:A:368:HIS:CE1	1:A:398:SER:HB3	2.49	0.47
1:A:458:SER:HB2	5:A:2715:HOH:O	2.10	0.47
1:A:587:THR:HG21	1:A:589:ASN:HD22	1.80	0.46
1:B:83:PRO:HD3	5:B:2162:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:MET:HB3	5:A:2504:HOH:O	2.13	0.46
1:A:121:PHE:HA	1:A:124:TRP:CD2	2.51	0.46
1:A:221:LEU:O	1:A:225:MET:HG2	2.15	0.46
1:B:118:HIS:NE2	1:B:129:ARG:NH2	2.63	0.46
1:A:39:THR:HB	5:A:2071:HOH:O	2.16	0.46
1:B:427:ARG:NH1	1:B:642:ASP:OD1	2.48	0.46
1:A:581:SER:HA	1:A:582:PRO:C	2.41	0.46
1:B:111:MET:HG2	1:B:240[B]:LEU:HD11	1.97	0.46
1:A:111:MET:HE2	1:A:188:GLY:HA2	1.98	0.45
1:A:523:ASN:ND2	1:A:526:GLY:H	2.13	0.45
1:A:46:ARG:HD3	1:A:295:ALA:C	2.41	0.45
1:A:240[B]:LEU:HD23	1:A:240[B]:LEU:HA	1.51	0.45
1:A:529:LYS:CE	5:A:2777:HOH:O	2.63	0.45
1:B:49:VAL:HG21	1:B:416:VAL:HG11	1.98	0.45
1:A:139:LYS:CE	1:A:542:THR:HG21	2.44	0.45
1:A:289:PRO:HD3	2:A:700:HEC:CAD	2.47	0.45
1:A:111:MET:CE	1:A:225:MET:HE3	2.42	0.45
1:A:292:TRP:CD2	1:A:348:PRO:HA	2.52	0.45
1:A:459:TRP:HA	5:A:2716:HOH:O	2.17	0.45
1:B:121:PHE:HA	1:B:124:TRP:CD2	2.52	0.44
1:A:139:LYS:HE2	1:A:542:THR:HG23	1.97	0.44
1:B:421:THR:O	1:B:500:GLY:HA3	2.17	0.44
1:A:257:LEU:CD1	1:A:604:ALA:HB2	2.47	0.44
1:A:70:LEU:HD22	1:A:492:PRO:HG2	2.00	0.44
1:B:257:LEU:CD1	1:B:604:ALA:HB2	2.48	0.44
1:B:434:ARG:HH11	1:B:434:ARG:HG3	1.82	0.44
1:B:656:ILE:O	1:B:660:LYS:HG3	2.18	0.44
1:A:147:PRO:HG3	1:A:207:PHE:CG	2.53	0.44
1:A:116:SER:HB3	1:A:228:THR:HB	2.00	0.43
1:A:300:GLN:NE2	2:A:700:HEC:HAA1	2.32	0.43
1:A:353:LYS:HE3	1:A:562:TRP:CE2	2.53	0.43
1:A:434:ARG:HH11	1:A:434:ARG:HG3	1.83	0.43
1:B:108:PHE:CE1	1:B:240[B]:LEU:CD2	3.02	0.43
1:B:576:ASN:ND2	1:B:590:MET:HG3	2.34	0.43
1:A:523:ASN:HD22	1:A:526:GLY:H	1.67	0.43
1:B:292:TRP:CD2	1:B:348:PRO:HA	2.53	0.43
1:A:15:ALA:N	5:A:2001:HOH:O	2.52	0.42
1:B:397:TYR:CE1	1:B:415:GLY:HA2	2.54	0.42
1:B:425:THR:CG2	5:B:2347:HOH:O	2.65	0.42
1:B:111:MET:HG2	1:B:240[B]:LEU:HD12	1.99	0.42
1:A:437:ALA:C	1:A:442[A]:ARG:HH12	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ASP:HB3	1:B:184:THR:HG22	2.02	0.42
1:B:314:GLU:OE2	1:B:340:ASN:ND2	2.52	0.42
1:A:535:LYS:C	1:A:536:LEU:HD12	2.44	0.42
1:B:250:ASP:O	1:B:251:ALA:C	2.62	0.42
1:B:331:GLY:HA3	5:B:2554:HOH:O	2.20	0.42
1:A:454:ASN:HA	1:A:459:TRP:CG	2.55	0.42
1:A:460:THR:HG23	1:A:461:GLY:N	2.34	0.42
1:B:108:PHE:CZ	1:B:240[B]:LEU:CD2	2.97	0.42
1:A:408:LEU:HD22	1:A:409:PRO:HD2	2.01	0.42
1:A:587:THR:HB	1:A:589:ASN:N	2.34	0.42
1:B:289:PRO:HD3	2:B:700:HEC:CAD	2.50	0.42
1:B:300:GLN:O	1:B:301:PHE:HB2	2.19	0.41
1:B:588:HIS:CB	5:B:2791:HOH:O	2.56	0.41
1:A:428:THR:O	1:A:429:ASP:C	2.64	0.41
1:A:476:PRO:HB2	1:A:487:TYR:CG	2.55	0.41
1:B:300:GLN:NE2	2:B:700:HEC:HAA1	2.35	0.41
1:A:35:LYS:HB3	1:A:39:THR:CG2	2.35	0.41
1:A:529:LYS:HD2	1:A:652:ARG:NH1	2.35	0.41
1:B:68:VAL:HB	1:B:307:SER:HB2	2.02	0.41
1:B:380:ALA:HB3	5:B:2609:HOH:O	2.21	0.41
1:B:587:THR:HB	1:B:589:ASN:H	1.86	0.40
1:B:351:TYR:HA	1:B:352:PRO:HD3	1.87	0.40
1:B:382:PRO:O	1:B:425:THR:HB	2.21	0.40
4:A:1664:EPE:H61	4:A:1664:EPE:H102	1.89	0.40
1:B:111:MET:CG	1:B:240[B]:LEU:HD13	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	650/662 (98%)	631 (97%)	18 (3%)	1 (0%)	43 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	651/662 (98%)	632 (97%)	18 (3%)	1 (0%)	43	31
All	All	1301/1324 (98%)	1263 (97%)	36 (3%)	2 (0%)	43	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	461	GLY
1	B	461	GLY

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	536/541 (99%)	509 (95%)	27 (5%)	22	10
1	B	537/541 (99%)	510 (95%)	27 (5%)	22	10
All	All	1073/1082 (99%)	1019 (95%)	54 (5%)	22	10

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	39	THR
1	A	50	LYS
1	A	206	SER
1	A	208	LYS
1	A	237	LEU
1	A	240[A]	LEU
1	A	240[B]	LEU
1	A	254	LEU
1	A	261	LEU
1	A	300	GLN
1	A	310	ASN
1	A	322	ILE
1	A	387	ASN

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Mol	Chain	Res	Type
1	A	398	SER
1	A	408	LEU
1	A	425	THR
1	A	454	ASN
1	A	460	THR
1	A	472	LEU
1	A	523	ASN
1	A	524	LEU
1	A	529	LYS
1	A	542	THR
1	A	565	LEU
1	A	578	ILE
1	A	587	THR
1	B	39	THR
1	B	108	PHE
1	B	211	LEU
1	B	240[A]	LEU
1	B	240[B]	LEU
1	B	261	LEU
1	B	300	GLN
1	B	310	ASN
1	B	322	ILE
1	B	327	ASN
1	B	354	THR
1	B	362	GLN
1	B	370	ARG
1	B	387	ASN
1	B	398	SER
1	B	425	THR
1	B	427	ARG
1	B	454	ASN
1	B	458	SER
1	B	467	ILE
1	B	472	LEU
1	B	523	ASN
1	B	524	LEU
1	B	565	LEU
1	B	578	ILE
1	B	587	THR
1	B	642	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	54	ASN
1	A	136	GLN
1	A	150	ASN
1	A	163	ASN
1	A	180	ASN
1	A	300	GLN
1	A	362	GLN
1	A	387	ASN
1	A	453	ASN
1	A	454	ASN
1	A	466	ASN
1	A	481	ASN
1	A	523	ASN
1	A	576	ASN
1	A	589	ASN
1	A	602	ASN
1	A	609	ASN
1	A	613	GLN
1	B	54	ASN
1	B	136	GLN
1	B	150	ASN
1	B	163	ASN
1	B	300	GLN
1	B	340	ASN
1	B	387	ASN
1	B	454	ASN
1	B	466	ASN
1	B	482	ASN
1	B	523	ASN
1	B	589	ASN
1	B	602	ASN
1	B	613	GLN
1	B	621	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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
2	HEC	B	701	1	46,50,50	2.51	21 (45%)	58,82,82	2.31	21 (36%)
4	EPE	A	1664	-	15,15,15	2.28	2 (13%)	19,20,20	1.06	2 (10%)
4	EPE	B	1664	-	15,15,15	2.28	2 (13%)	19,20,20	1.79	5 (26%)
3	OXY	B	1663	2	1,1,1	0.60	0	-		
2	HEC	A	701	1	46,50,50	2.39	18 (39%)	58,82,82	2.23	18 (31%)
3	OXY	A	1663	2	1,1,1	0.63	0	-		
2	HEC	B	700	3,1	46,50,50	2.31	24 (52%)	58,82,82	2.21	21 (36%)
2	HEC	A	700	3,1	46,50,50	2.33	19 (41%)	58,82,82	2.35	29 (50%)

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
2	HEC	B	701	1	-	4/14/54/54	-
4	EPE	A	1664	-	-	5/9/19/19	0/1/1/1
4	EPE	B	1664	-	-	2/9/19/19	0/1/1/1
2	HEC	A	701	1	-	6/14/54/54	-
2	HEC	B	700	3,1	-	6/14/54/54	-
2	HEC	A	700	3,1	-	7/14/54/54	-

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1664	EPE	C10-S	-6.34	1.68	1.77
4	A	1664	EPE	C10-S	-5.90	1.69	1.77
4	A	1664	EPE	O3S-S	5.80	1.69	1.47
2	B	701	HEC	C2A-C3A	5.69	1.49	1.36
4	B	1664	EPE	O2S-S	5.67	1.61	1.45
2	A	701	HEC	CAB-C3B	5.19	1.51	1.35
2	A	701	HEC	C2A-C3A	5.15	1.47	1.36
2	A	700	HEC	C4D-ND	-4.95	1.30	1.39
2	A	700	HEC	CAB-C3B	4.95	1.51	1.35
2	A	701	HEC	CAC-C3C	4.75	1.50	1.35
2	A	700	HEC	CAC-C3C	4.70	1.50	1.35
2	B	701	HEC	CHB-C4A	4.55	1.47	1.38
2	B	700	HEC	CAC-C3C	4.40	1.49	1.35
2	B	701	HEC	CHD-C4C	4.24	1.46	1.38
2	B	701	HEC	CAB-C3B	4.12	1.48	1.35
2	B	701	HEC	CHC-C4B	4.07	1.46	1.38
2	A	700	HEC	CHC-C4B	4.06	1.46	1.38
2	B	701	HEC	CAC-C3C	4.04	1.48	1.35
2	A	701	HEC	CHC-C4B	3.96	1.46	1.38
2	A	701	HEC	CBC-CAC	-3.89	1.35	1.49
2	B	701	HEC	C1D-ND	-3.83	1.32	1.39
2	A	700	HEC	CHA-C1A	3.82	1.45	1.38
2	B	700	HEC	CHD-C1D	3.78	1.47	1.39
2	B	700	HEC	CAB-C3B	3.77	1.47	1.35
2	B	701	HEC	C1B-NB	-3.74	1.32	1.39
2	A	700	HEC	CHD-C4C	3.69	1.45	1.38
2	A	701	HEC	CHD-C1D	3.68	1.47	1.39
2	B	700	HEC	C2A-C3A	3.67	1.44	1.36
2	B	701	HEC	CBB-CAB	-3.60	1.36	1.49
2	B	701	HEC	CBC-CAC	-3.54	1.36	1.49
2	B	701	HEC	C4A-NA	3.51	1.46	1.39
2	A	700	HEC	C4C-NC	3.47	1.46	1.39
2	A	701	HEC	C4A-NA	3.42	1.46	1.39
2	B	700	HEC	CHD-C4C	3.41	1.45	1.38
2	A	701	HEC	C1D-ND	-3.36	1.33	1.39
2	B	700	HEC	CBB-CAB	-3.34	1.37	1.49
2	A	701	HEC	CHA-C1A	3.33	1.44	1.38
2	B	701	HEC	C1C-NC	3.28	1.45	1.39
2	A	701	HEC	CHD-C4C	3.24	1.44	1.38
2	A	700	HEC	CHD-C1D	3.24	1.46	1.39
2	B	700	HEC	C3D-C2D	3.20	1.47	1.38
2	A	700	HEC	C1D-ND	-3.17	1.33	1.39
2	A	701	HEC	C1B-NB	-3.15	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	HEC	CHB-C4A	3.13	1.44	1.38
2	B	700	HEC	CHC-C4B	3.03	1.44	1.38
2	A	700	HEC	C4A-NA	3.01	1.45	1.39
2	A	701	HEC	CHB-C1B	2.98	1.46	1.39
2	B	700	HEC	C1C-NC	2.97	1.45	1.39
2	B	700	HEC	C4A-NA	2.96	1.45	1.39
2	A	701	HEC	CHA-C4D	2.93	1.46	1.39
2	B	700	HEC	C1B-NB	-2.93	1.34	1.39
2	B	700	HEC	C1D-ND	-2.91	1.34	1.39
2	B	700	HEC	CHA-C1A	2.88	1.44	1.38
2	A	700	HEC	C2A-C3A	2.87	1.43	1.36
2	A	700	HEC	C1B-NB	-2.86	1.34	1.39
2	B	700	HEC	C4B-NB	-2.84	1.34	1.39
2	A	700	HEC	CHA-C4D	2.81	1.45	1.39
2	B	701	HEC	CHA-C1A	2.80	1.43	1.38
2	B	700	HEC	C1C-C2C	2.75	1.49	1.43
2	B	700	HEC	C4D-ND	-2.74	1.34	1.39
2	A	701	HEC	O2D-CGD	-2.73	1.21	1.30
2	B	700	HEC	CHA-C4D	2.73	1.45	1.39
2	B	700	HEC	C3C-C4C	-2.69	1.41	1.46
2	B	701	HEC	CHB-C1B	2.64	1.45	1.39
2	B	701	HEC	CHA-C4D	2.58	1.45	1.39
2	B	700	HEC	CHB-C1B	2.56	1.45	1.39
2	B	701	HEC	C1B-C2B	2.52	1.49	1.43
2	A	701	HEC	CBB-CAB	-2.50	1.40	1.49
2	A	700	HEC	CBC-CAC	-2.48	1.40	1.49
2	A	700	HEC	C1C-C2C	2.47	1.48	1.43
2	B	700	HEC	CHB-C4A	2.44	1.43	1.38
2	A	700	HEC	CHC-C1C	2.36	1.44	1.39
2	B	701	HEC	C3D-C2D	2.34	1.45	1.38
2	A	701	HEC	C3D-C2D	2.29	1.44	1.38
2	B	700	HEC	C4C-NC	2.29	1.43	1.39
2	B	701	HEC	C1A-C2A	2.28	1.49	1.45
2	B	700	HEC	O1A-CGA	2.27	1.29	1.22
2	B	700	HEC	CBC-CAC	-2.25	1.41	1.49
2	A	700	HEC	CHB-C1B	2.24	1.44	1.39
2	B	700	HEC	C4A-C3A	2.21	1.49	1.45
2	B	701	HEC	CHD-C1D	2.17	1.44	1.39
2	A	700	HEC	C3C-C2C	2.13	1.48	1.41
2	B	701	HEC	C1C-C2C	2.13	1.48	1.43
2	A	700	HEC	O2A-CGA	-2.10	1.23	1.30
2	B	701	HEC	C3C-C2C	2.10	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	HEC	C3B-C2B	2.01	1.48	1.41

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	HEC	CBB-CAB-C3B	-6.77	113.89	127.43
2	B	701	HEC	CBB-CAB-C3B	-6.63	114.19	127.43
2	A	700	HEC	CBB-CAB-C3B	-6.32	114.81	127.43
2	A	701	HEC	C3D-C4D-ND	5.75	116.54	110.15
2	B	701	HEC	CBC-CAC-C3C	-5.62	116.20	127.43
2	A	701	HEC	C2D-C1D-ND	5.02	118.19	110.14
2	B	701	HEC	C3D-C4D-ND	4.92	115.61	110.15
2	A	700	HEC	CBC-CAC-C3C	-4.87	117.70	127.43
2	B	700	HEC	C2B-C1B-NB	4.82	117.87	110.14
2	A	700	HEC	CBD-CAD-C3D	-4.82	99.20	112.53
2	B	700	HEC	C3D-C4D-ND	4.73	115.40	110.15
2	B	701	HEC	CBA-CAA-C2A	-4.52	100.03	112.53
2	A	700	HEC	CHC-C4B-C3B	-4.49	117.64	125.21
2	B	700	HEC	CBD-CAD-C3D	-4.27	100.72	112.53
2	B	700	HEC	CBC-CAC-C3C	-4.19	119.06	127.43
2	B	700	HEC	CBB-CAB-C3B	-4.10	119.23	127.43
2	A	701	HEC	CBA-CAA-C2A	-4.05	101.33	112.53
2	B	701	HEC	C2B-C1B-NB	3.98	116.52	110.14
2	A	700	HEC	CMD-C2D-C1D	3.94	131.42	125.42
2	B	700	HEC	CMA-C3A-C4A	3.90	131.59	124.73
2	A	701	HEC	C2B-C1B-NB	3.86	116.33	110.14
2	B	700	HEC	CAD-C3D-C4D	3.82	132.40	124.94
2	A	701	HEC	C1D-C2D-C3D	-3.79	102.48	106.82
2	B	701	HEC	C2D-C1D-ND	3.78	116.20	110.14
2	A	700	HEC	C2B-C1B-NB	3.70	116.07	110.14
2	A	700	HEC	C1D-C2D-C3D	-3.69	102.59	106.82
4	B	1664	EPE	C6-N1-C2	3.66	116.72	108.84
4	B	1664	EPE	O2S-S-C10	-3.63	101.24	106.73
2	B	700	HEC	C1D-C2D-C3D	-3.52	102.78	106.82
2	A	701	HEC	C4D-ND-C1D	-3.46	100.18	105.82
2	B	700	HEC	CMD-C2D-C1D	3.24	130.36	125.42
2	B	701	HEC	CMC-C2C-C1C	3.23	130.34	125.42
2	B	701	HEC	C2C-C1C-NC	3.22	115.30	110.14
2	A	701	HEC	O2A-CGA-CBA	3.22	124.16	114.00
2	A	700	HEC	CHB-C1B-C2B	-3.20	118.14	127.43
2	B	701	HEC	C4D-C3D-C2D	-3.19	101.93	106.87
2	A	700	HEC	CMB-C2B-C3B	3.19	134.05	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	HEC	C2A-C1A-NA	3.18	113.39	110.32
2	B	700	HEC	CHD-C1D-C2D	-3.16	118.25	127.43
2	A	701	HEC	CHD-C1D-C2D	-3.14	118.30	127.43
2	A	700	HEC	C4A-NA-C1A	-3.10	100.76	105.82
4	B	1664	EPE	O3S-S-C10	3.09	112.06	106.00
2	B	700	HEC	C2D-C1D-ND	3.09	115.10	110.14
2	B	701	HEC	CBD-CAD-C3D	-3.09	103.99	112.53
2	A	701	HEC	C2C-C1C-NC	3.07	115.06	110.14
2	B	701	HEC	CMB-C2B-C3B	3.06	133.75	126.55
2	B	700	HEC	CHD-C4C-C3C	-2.98	120.18	125.21
2	B	701	HEC	C1D-C2D-C3D	-2.98	103.40	106.82
2	B	700	HEC	CHC-C4B-C3B	-2.96	120.22	125.21
2	B	701	HEC	CHD-C1D-C2D	-2.94	118.89	127.43
2	A	700	HEC	CAD-C3D-C4D	2.92	130.64	124.94
2	A	701	HEC	C4D-C3D-C2D	-2.90	102.38	106.87
4	B	1664	EPE	C6-C5-N4	-2.87	104.87	110.65
2	B	700	HEC	CAA-CBA-CGA	-2.86	106.08	113.67
2	A	701	HEC	CAD-C3D-C4D	2.81	130.43	124.94
2	A	701	HEC	CBD-CAD-C3D	-2.81	104.76	112.53
2	A	700	HEC	C4B-NB-C1B	-2.80	101.26	105.82
2	B	700	HEC	CHB-C1B-C2B	-2.75	119.44	127.43
2	B	700	HEC	C4D-C3D-C2D	-2.75	102.62	106.87
2	B	700	HEC	CBA-CAA-C2A	-2.65	105.20	112.53
2	B	701	HEC	CAA-CBA-CGA	-2.60	106.76	113.67
2	A	700	HEC	C3A-C4A-NA	2.60	114.44	109.64
2	B	701	HEC	CMD-C2D-C3D	2.59	131.12	125.62
2	A	700	HEC	CHA-C1A-C2A	-2.59	120.77	124.86
2	B	701	HEC	C2A-C1A-NA	2.59	112.82	110.32
2	A	700	HEC	CHD-C1D-C2D	-2.48	120.24	127.43
2	A	701	HEC	CMA-C3A-C4A	2.40	128.96	124.73
2	B	700	HEC	C4B-NB-C1B	-2.40	101.91	105.82
2	A	701	HEC	CHA-C4D-C3D	-2.35	120.15	125.30
2	B	701	HEC	CHB-C1B-C2B	-2.35	120.61	127.43
2	A	700	HEC	CBA-CAA-C2A	-2.33	106.08	112.53
2	A	700	HEC	CAA-C2A-C3A	-2.33	123.50	127.87
2	A	701	HEC	CMD-C2D-C1D	2.32	128.96	125.42
2	A	700	HEC	CHC-C4B-NB	2.31	126.96	124.45
2	B	700	HEC	C2A-C1A-NA	2.30	112.54	110.32
2	B	701	HEC	CHB-C4A-C3A	-2.29	120.72	125.49
2	B	700	HEC	CMB-C2B-C3B	2.25	131.85	126.55
2	A	700	HEC	C2D-C1D-ND	2.25	113.75	110.14
2	B	701	HEC	C3A-C4A-NA	2.25	113.80	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	HEC	C4D-CHA-C1A	-2.24	117.75	124.66
2	A	700	HEC	CHD-C4C-C3C	-2.23	121.44	125.21
2	A	700	HEC	CMA-C3A-C4A	2.23	128.66	124.73
2	B	700	HEC	C4C-NC-C1C	-2.17	102.28	105.82
2	B	701	HEC	CHA-C4D-C3D	-2.17	120.56	125.30
2	A	700	HEC	C2C-C1C-NC	2.15	113.59	110.14
2	B	701	HEC	C4A-C3A-C2A	-2.13	103.81	106.97
2	A	701	HEC	CHC-C4B-C3B	-2.12	121.63	125.21
2	A	700	HEC	C4A-C3A-C2A	-2.11	103.85	106.97
4	A	1664	EPE	O3S-S-C10	2.08	110.08	106.00
4	B	1664	EPE	C3-C2-N1	2.08	114.85	110.65
2	A	700	HEC	CMC-C2C-C3C	2.08	131.43	126.55
2	A	700	HEC	CHC-C1C-NC	-2.06	120.13	123.86
2	A	700	HEC	CHA-C4D-C3D	-2.03	120.85	125.30
2	A	700	HEC	CAA-C2A-C1A	2.03	128.97	124.85
4	A	1664	EPE	O2S-S-O1S	-2.01	107.27	113.82
2	A	701	HEC	C4C-NC-C1C	-2.00	102.56	105.82

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700	HEC	C2B-C3B-CAB-CBB
2	A	700	HEC	C4B-C3B-CAB-CBB
2	A	700	HEC	C2C-C3C-CAC-CBC
2	A	700	HEC	C4C-C3C-CAC-CBC
2	A	701	HEC	C2B-C3B-CAB-CBB
2	A	701	HEC	C4B-C3B-CAB-CBB
2	A	701	HEC	C2C-C3C-CAC-CBC
2	A	701	HEC	C4C-C3C-CAC-CBC
2	B	700	HEC	C2B-C3B-CAB-CBB
2	B	700	HEC	C4B-C3B-CAB-CBB
2	B	700	HEC	C2C-C3C-CAC-CBC
2	B	700	HEC	C4C-C3C-CAC-CBC
2	B	701	HEC	C2B-C3B-CAB-CBB
2	B	701	HEC	C4B-C3B-CAB-CBB
2	B	701	HEC	C2C-C3C-CAC-CBC
2	B	701	HEC	C4C-C3C-CAC-CBC
4	A	1664	EPE	C10-C9-N1-C6
4	A	1664	EPE	C8-C7-N4-C3
4	A	1664	EPE	N4-C7-C8-O8
4	B	1664	EPE	C8-C7-N4-C5

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Mol	Chain	Res	Type	Atoms
4	B	1664	EPE	N4-C7-C8-O8
4	A	1664	EPE	C10-C9-N1-C2
4	A	1664	EPE	S-C10-C9-N1
2	A	700	HEC	CAD-CBD-CGD-O1D
2	A	700	HEC	CAD-CBD-CGD-O2D
2	B	700	HEC	CAD-CBD-CGD-O2D
2	A	701	HEC	CAD-CBD-CGD-O1D
2	B	700	HEC	CAD-CBD-CGD-O1D
2	A	701	HEC	CAD-CBD-CGD-O2D
2	A	700	HEC	CAA-CBA-CGA-O1A

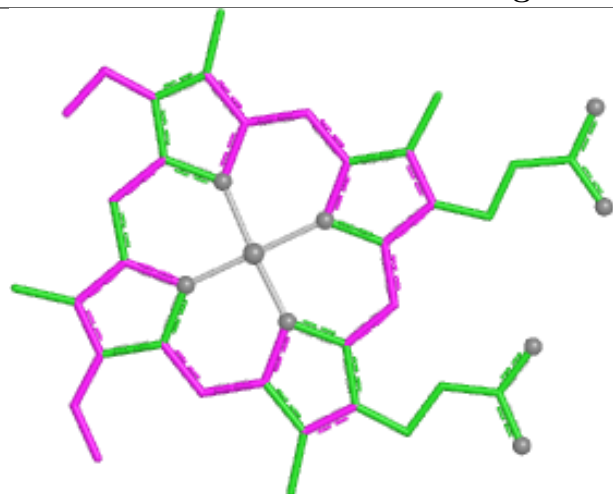
There are no ring outliers.

5 monomers are involved in 12 short contacts:

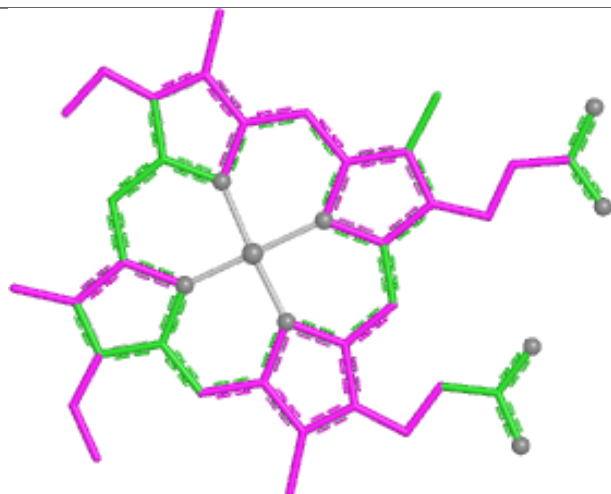
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	HEC	4	0
4	A	1664	EPE	1	0
2	A	701	HEC	1	0
2	B	700	HEC	3	0
2	A	700	HEC	3	0

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.

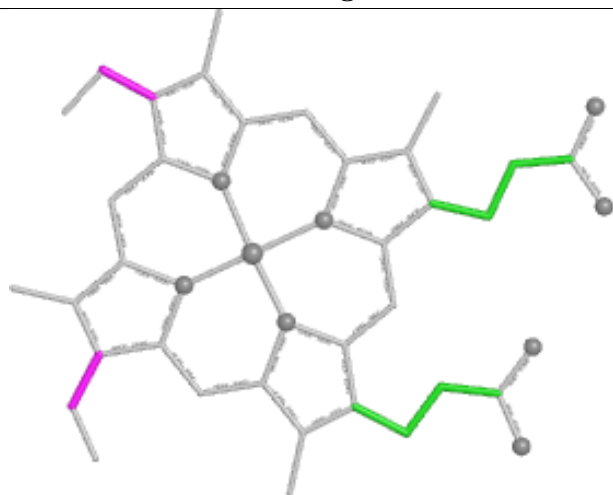
Ligand HEC B 701



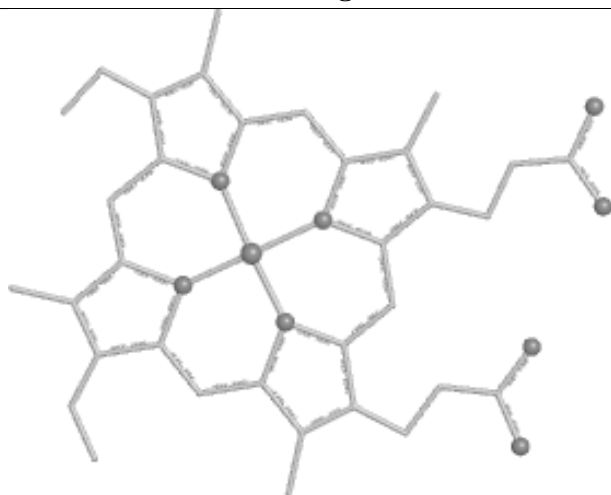
Bond lengths



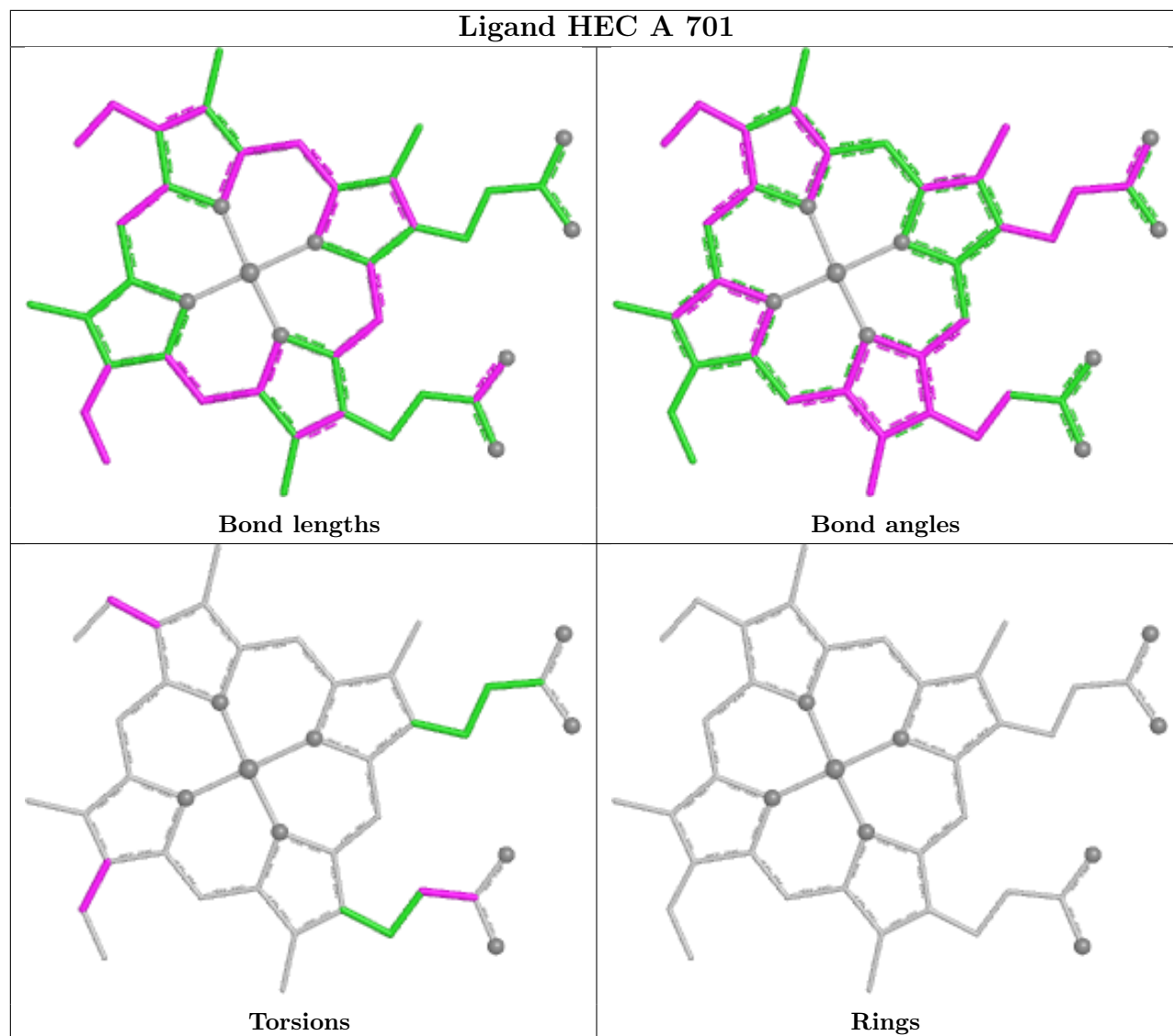
Bond angles



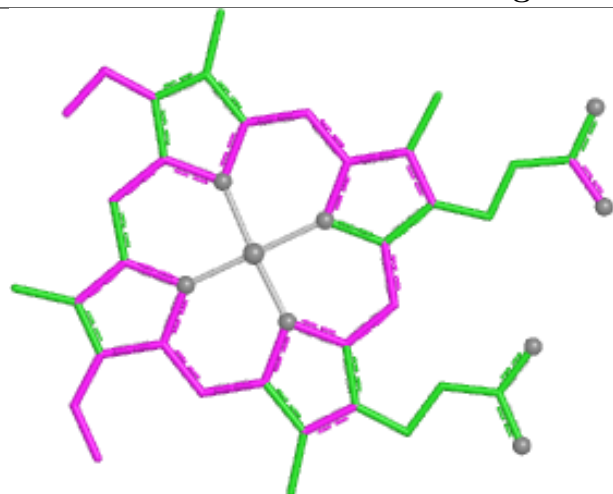
Torsions



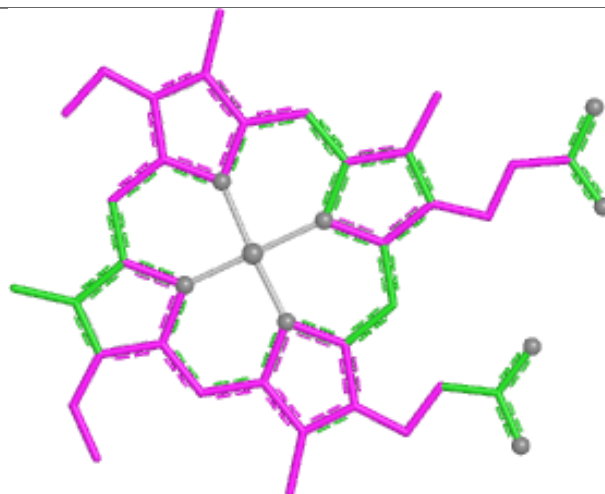
Rings



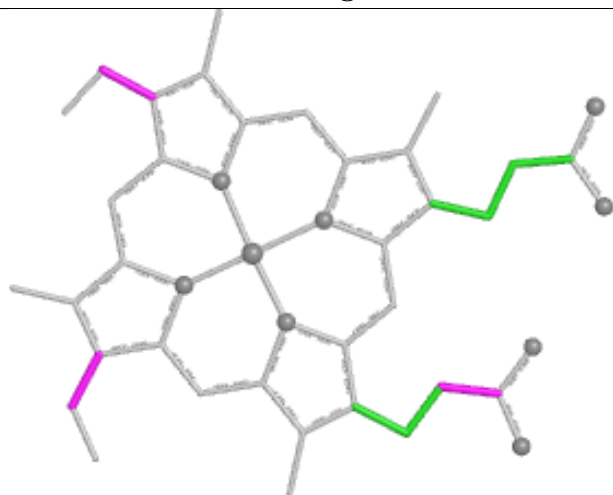
Ligand HEC B 700



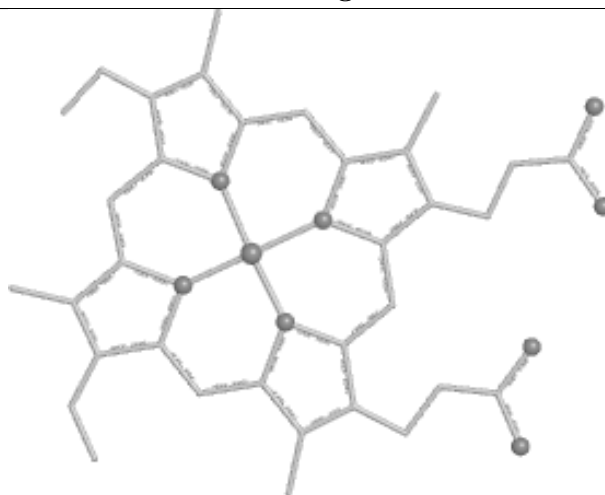
Bond lengths



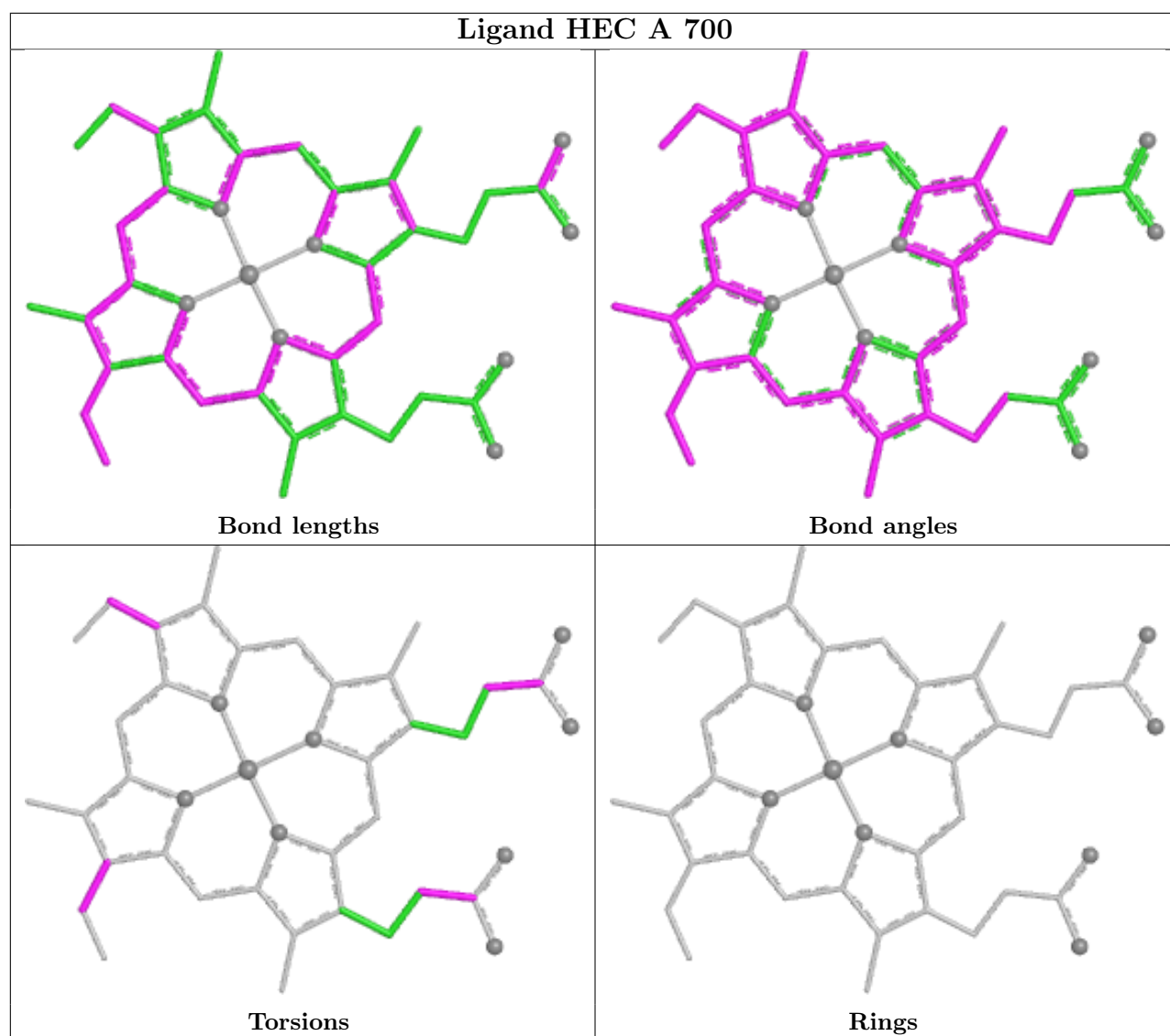
Bond angles



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	648/662 (97%)	-0.49	1 (0%) 91 91	9, 19, 33, 51	4 (0%)
1	B	648/662 (97%)	-0.41	2 (0%) 90 90	9, 22, 37, 53	5 (0%)
All	All	1296/1324 (97%)	-0.45	3 (0%) 91 91	9, 20, 35, 53	9 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	460	THR	2.6
1	A	234	LEU	2.5
1	B	15	ALA	2.1

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.

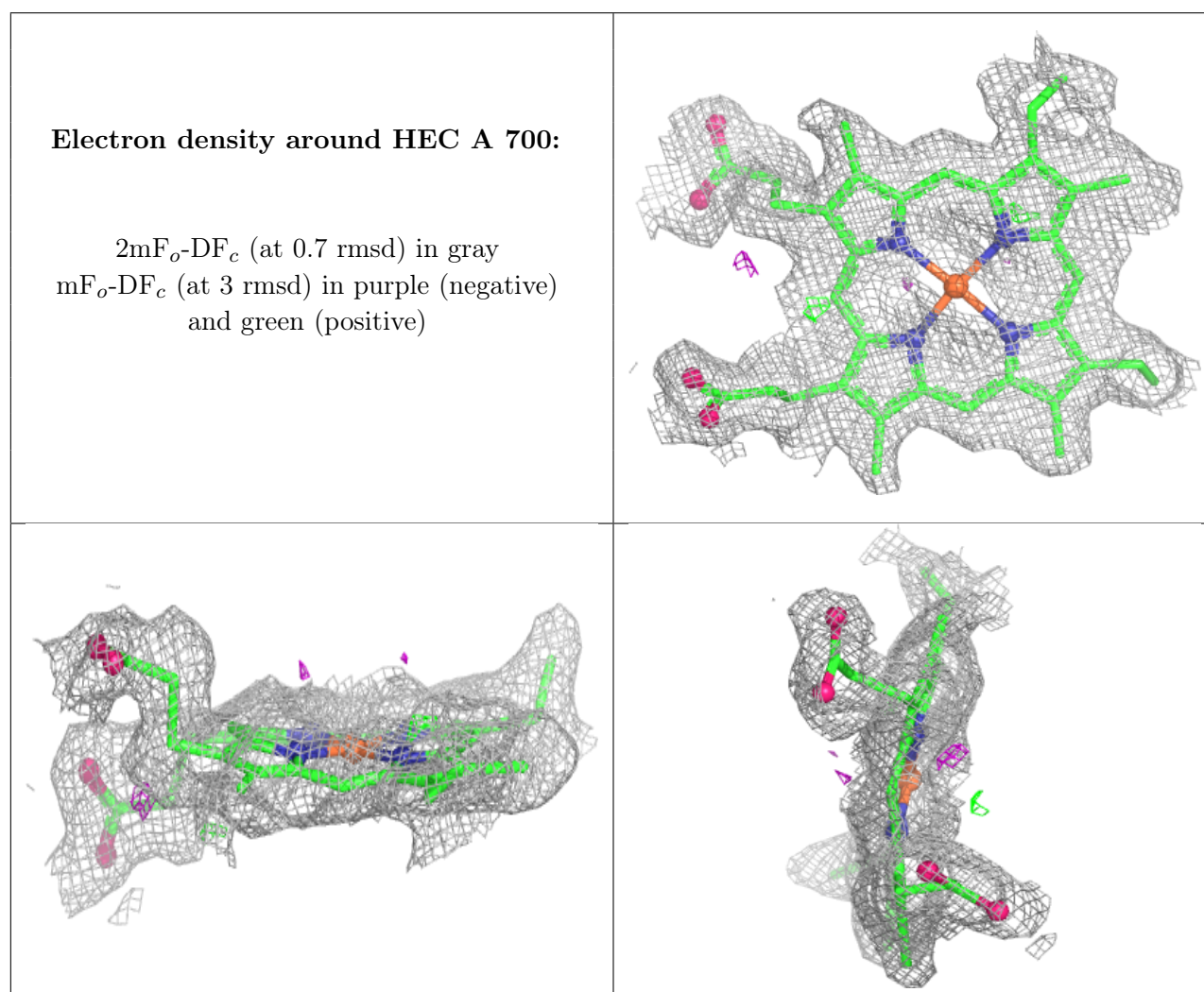
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EPE	A	1664	15/15	0.88	0.14	37,51,66,78	0
4	EPE	B	1664	15/15	0.94	0.09	25,36,55,66	0

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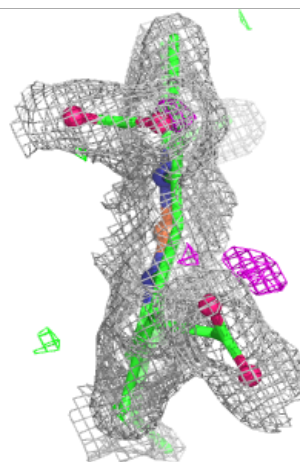
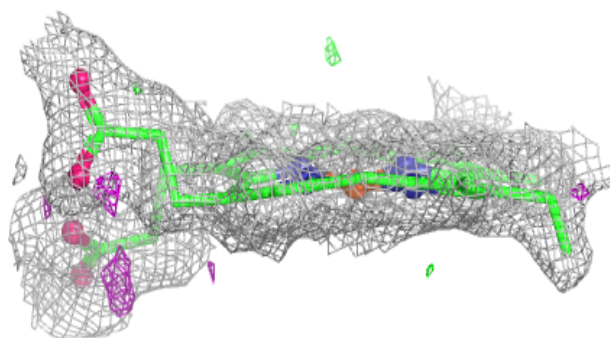
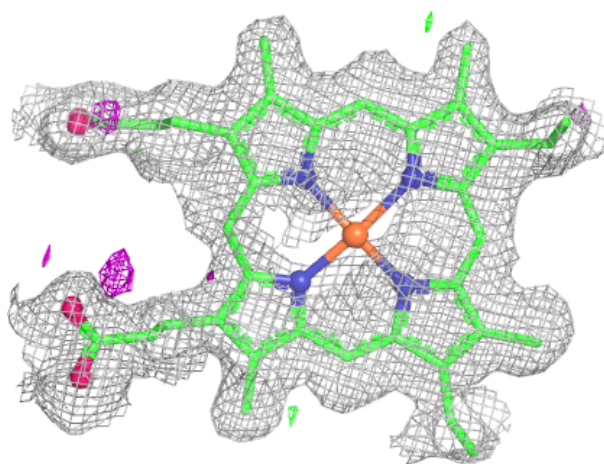
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	OXY	A	1663	2/2	0.97	0.08	19,19,19,30	0
3	OXY	B	1663	2/2	0.97	0.12	25,25,25,35	0
2	HEC	A	700	43/43	0.99	0.04	11,12,14,15	0
2	HEC	A	701	43/43	0.99	0.04	14,18,19,22	0
2	HEC	B	700	43/43	0.99	0.04	12,14,15,16	0
2	HEC	B	701	43/43	0.99	0.05	17,20,24,25	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.



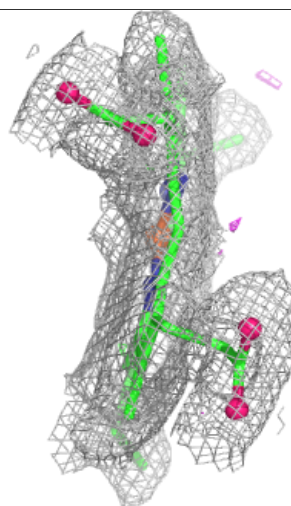
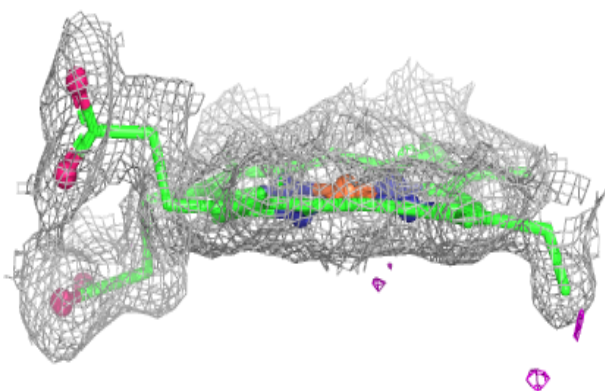
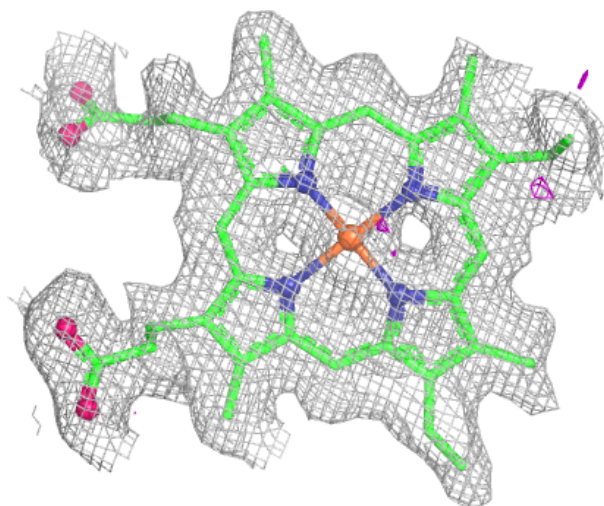
Electron density around HEC A 701:

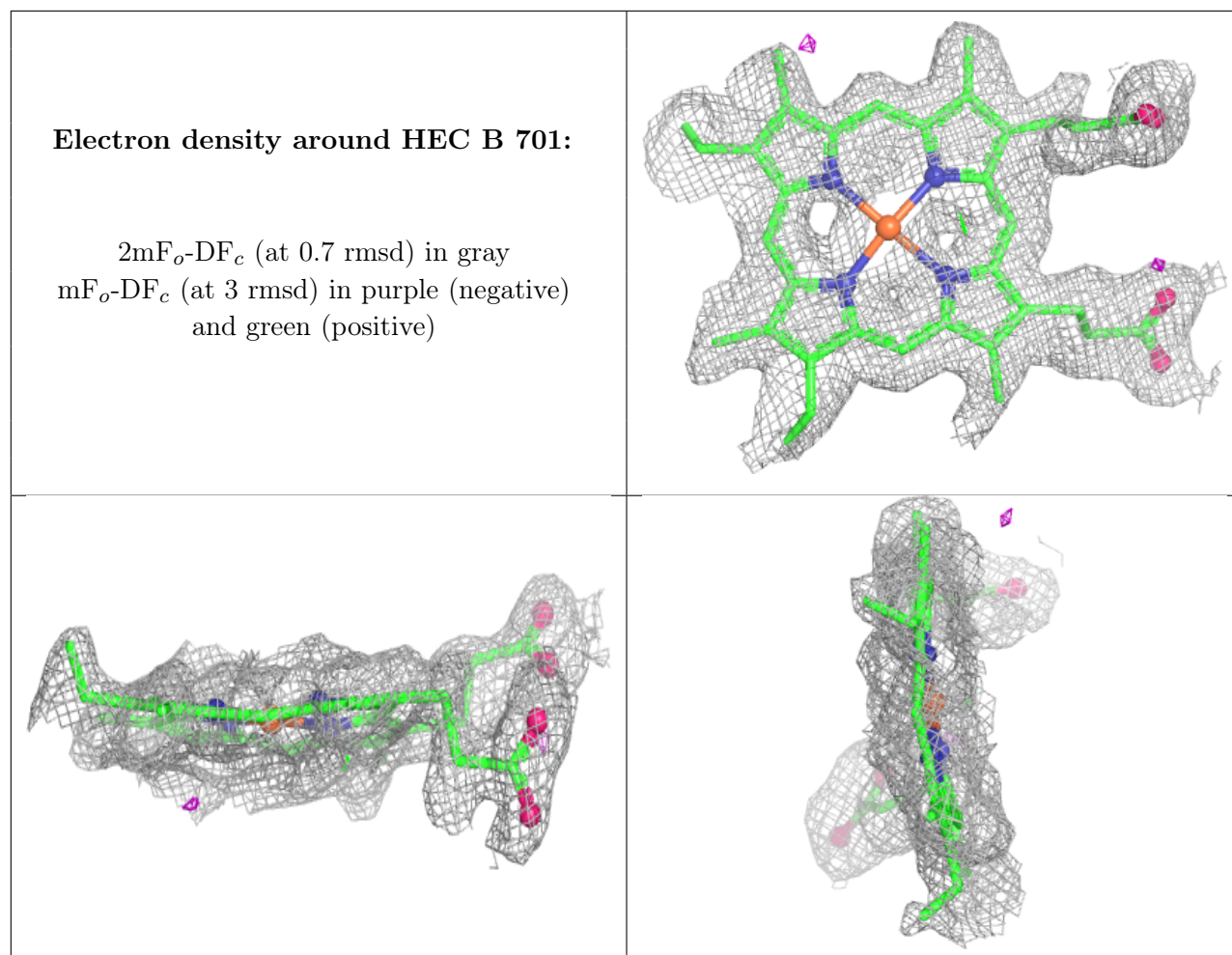
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC B 700:

$2mF_o-DF_c$ (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.