



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2024 – 09:14 PM EDT

PDB ID : 1NIR  
Title : OXYDIZED NITRITE REDUCTASE FROM PSEUDOMONAS AERUGINOSA  
Authors : Nurizzo, D.; Tegoni, M.; Cambillau, C.  
Deposited on : 1997-06-17  
Resolution : 2.15 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](mailto: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>.

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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 : 2.36.1  
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) : 2.36.1

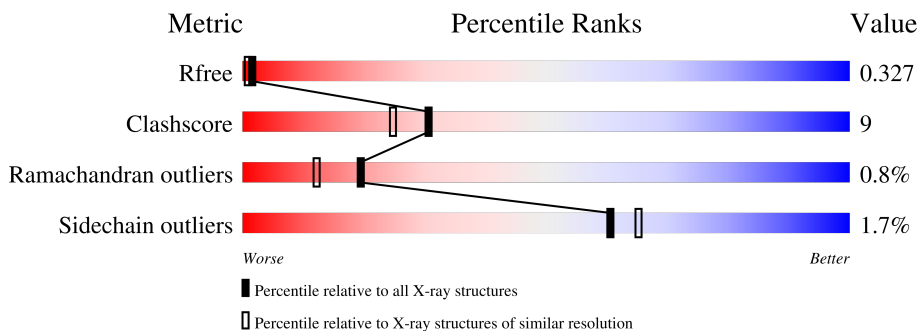
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	543	75% 22% ...
1	B	543	79% 18% ...

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
2	PO4	A	604	-	X	-	-
2	PO4	B	604	-	X	-	-
6	DHE	A	602	X	-	-	-

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
6	DHE	B	602	X	-	-	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9483 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 NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	538	Total 4203	C 2665	N 733	O 793	S 12	0	0	0
1	B	539	Total 4212	C 2671	N 735	O 794	S 12	0	0	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

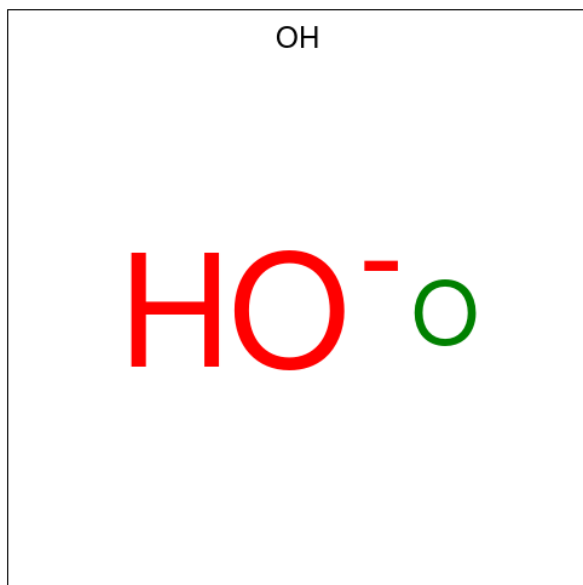


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



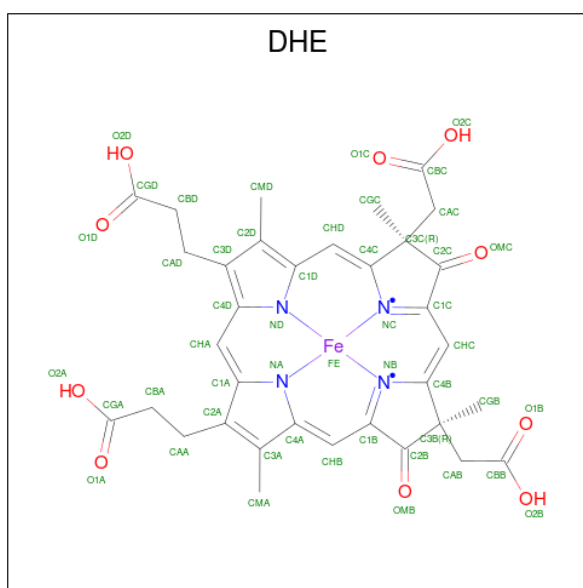
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	B	1	Total O 1 1	0	0

- Molecule 5 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 6 is HEME D (three-letter code: DHE) (formula:  $C_{34}H_{32}FeN_4O_{10}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	A	1	Total	C	Fe	N	O	0	0
			49	34	1	4	10		
6	B	1	Total	C	Fe	N	O	0	0
			49	34	1	4	10		

- Molecule 7 is water.

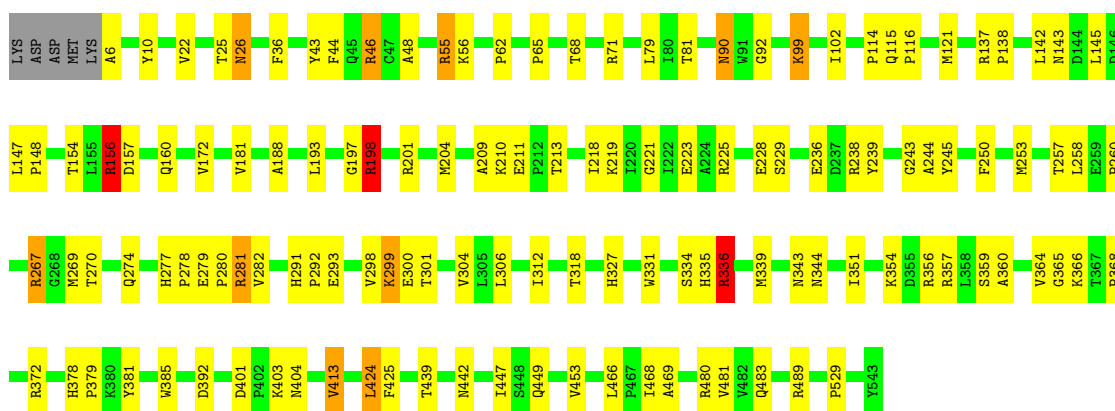
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	449	Total 449	O 449	0	0
7	B	421	Total 421	O 421	0	0

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

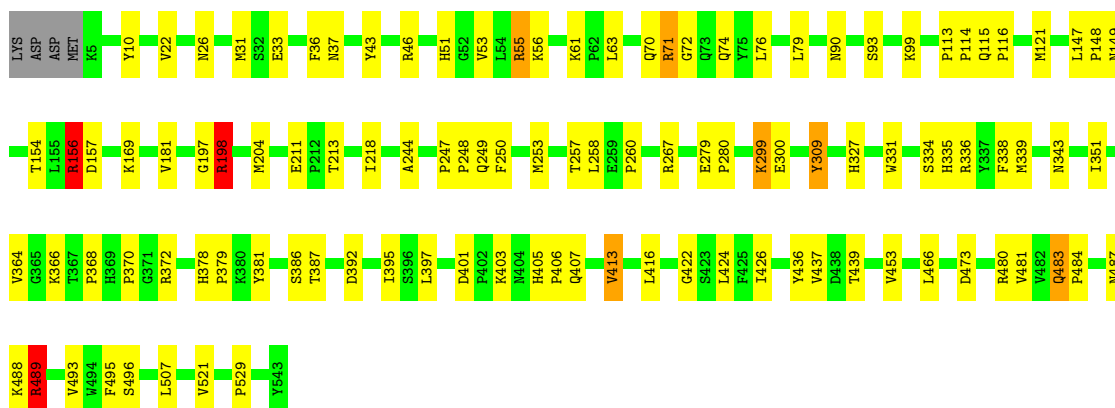
- Molecule 1: NITRITE REDUCTASE

Chain A:  75% 22% ...



- Molecule 1: NITRITE REDUCTASE

Chain B:  79% 18% ...





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.07Å 90.07Å 111.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.15 29.48 – 2.13	Depositor EDS
% Data completeness (in resolution range)	89.0 (30.00-2.15) 88.7 (29.48-2.13)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.31 (at 2.14Å)	Xtrriage
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.209 , 0.242 0.318 , 0.327	Depositor DCC
$R_{free}$ test set	3270 reflections (3.57%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.2	Xtrriage
Anisotropy	0.053	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 34.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	9483	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.9823e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.79	1/4308 (0.0%)	1.03	21/5854 (0.4%)
1	B	0.67	2/4317 (0.0%)	0.91	15/5865 (0.3%)
All	All	0.73	3/8625 (0.0%)	0.97	36/11719 (0.3%)

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
1	B	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	248	PRO	C-N	-6.38	1.19	1.34
1	B	244	ALA	C-N	-5.06	1.22	1.34
1	A	244	ALA	C-N	-5.02	1.22	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	ARG	NE-CZ-NH2	7.62	124.11	120.30
1	B	489	ARG	NE-CZ-NH2	7.59	124.09	120.30
1	A	156	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	A	267	ARG	NE-CZ-NH2	7.49	124.05	120.30
1	A	238	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	B	156	ARG	NE-CZ-NH2	7.45	124.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	B	480	ARG	NE-CZ-NH2	7.41	124.01	120.30
1	B	336	ARG	NE-CZ-NH2	7.37	123.98	120.30
1	B	372	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	A	372	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	A	225	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	A	55	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	A	46	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	A	336	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	A	356	ARG	NE-CZ-NH2	7.01	123.80	120.30
1	A	137	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	A	357	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	B	55	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	A	480	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	B	71	ARG	NE-CZ-NH2	6.77	123.68	120.30
1	A	489	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	A	71	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	B	198	ARG	NE-CZ-NH2	6.33	123.46	120.30
1	B	46	ARG	NE-CZ-NH2	6.17	123.39	120.30
1	A	253	MET	CG-SD-CE	6.16	110.05	100.20
1	B	339	MET	CG-SD-CE	6.13	110.00	100.20
1	B	253	MET	CG-SD-CE	6.11	109.97	100.20
1	A	204	MET	CG-SD-CE	6.08	109.93	100.20
1	A	269	MET	CG-SD-CE	6.06	109.90	100.20
1	B	309	TYR	O-C-N	-6.00	113.10	122.70
1	B	31	MET	CG-SD-CE	5.99	109.78	100.20
1	A	339	MET	CG-SD-CE	5.93	109.69	100.20
1	B	244	ALA	O-C-N	-5.77	113.46	122.70
1	B	204	MET	CG-SD-CE	5.36	108.77	100.20
1	A	198	ARG	NE-CZ-NH2	-5.19	117.70	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	385	TRP	Mainchain
1	B	309	TYR	Mainchain
1	B	483	GLN	Mainchain

## 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	4203	0	4157	86	0
1	B	4212	0	4169	76	2
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	43	0	30	1	0
5	B	43	0	30	3	0
6	A	49	0	24	3	0
6	B	49	0	24	3	0
7	A	449	0	0	5	1
7	B	421	0	0	7	2
All	All	9483	0	8434	157	5

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 9.

All (157) 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:488:LYS:HB3	7:B:1008:HOH:O	1.62	0.98
1:A:277:HIS:O	1:A:280:PRO:HD3	1.84	0.78
1:A:114:PRO:HB2	1:B:22:VAL:HG12	1.64	0.78
1:B:211:GLU:O	1:B:213:THR:HG23	1.87	0.75
1:B:489:ARG:HG2	7:B:1008:HOH:O	1.88	0.73
1:A:257:THR:O	1:A:258:LEU:HB2	1.88	0.72
1:A:364:VAL:CG2	1:A:368:PRO:HG3	2.21	0.70
1:A:22:VAL:HG12	1:B:114:PRO:HB2	1.75	0.68
1:A:278:PRO:HG3	7:A:947:HOH:O	1.93	0.67
1:A:219:LYS:HE3	1:A:221:GLY:O	1.95	0.67
1:A:147:LEU:HB2	1:A:148:PRO:HD3	1.77	0.66
1:A:43:TYR:OH	1:A:55:ARG:HG2	1.96	0.66
1:B:364:VAL:CG2	1:B:368:PRO:HG3	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:TYR:OH	1:B:327:HIS:HE1	1.81	0.63
1:B:487:ASN:HD21	1:B:489:ARG:HG3	1.63	0.63
1:B:401:ASP:HB3	1:B:405:HIS:HB2	1.81	0.63
1:B:257:THR:O	1:B:258:LEU:HB2	1.99	0.62
1:A:228:GLU:HG3	1:A:229:SER:N	2.15	0.60
1:B:343:ASN:HA	1:B:368:PRO:HD2	1.82	0.60
1:B:489:ARG:HD2	7:B:815:HOH:O	2.00	0.60
1:B:395:ILE:HB	1:B:416:LEU:HB2	1.82	0.60
1:B:484:PRO:HB3	1:B:495:PHE:CE2	2.37	0.60
1:A:55:ARG:NH2	7:A:789:HOH:O	2.29	0.59
1:A:364:VAL:HG21	1:A:368:PRO:HG3	1.84	0.59
1:A:36:PHE:HZ	1:A:114:PRO:HG3	1.67	0.59
1:A:90:ASN:H	1:A:90:ASN:HD22	1.50	0.59
1:A:25:THR:O	1:A:26:ASN:HB2	2.03	0.58
1:B:53:VAL:HG11	1:B:116:PRO:HG2	1.85	0.58
1:A:304:VAL:HG11	1:A:351:ILE:HG12	1.86	0.57
1:B:99:LYS:HD3	1:B:99:LYS:O	2.04	0.57
1:B:507:LEU:HB2	1:B:521:VAL:HB	1.86	0.57
1:A:364:VAL:HG23	1:A:368:PRO:HG3	1.86	0.56
1:A:279:GLU:O	1:A:279:GLU:HG2	2.04	0.56
1:A:291:HIS:O	1:A:293:GLU:N	2.38	0.56
1:A:327:HIS:HE1	1:B:10:TYR:OH	1.88	0.56
1:A:211:GLU:O	1:A:213:THR:HG23	2.06	0.55
1:B:55:ARG:NH2	7:B:693:HOH:O	2.27	0.55
1:B:61:LYS:HD2	1:B:71:ARG:NH2	2.22	0.55
5:A:601:HEC:HMC1	5:A:601:HEC:HBC3	1.87	0.55
1:A:366:LYS:HE3	1:A:392:ASP:OD2	2.08	0.54
1:B:453:VAL:HG21	1:B:466:LEU:HD22	1.90	0.53
1:A:90:ASN:H	1:A:90:ASN:ND2	2.07	0.53
1:B:364:VAL:HG21	1:B:368:PRO:HG3	1.91	0.53
1:A:381:TYR:CD1	1:A:413:VAL:HG22	2.43	0.53
1:B:198:ARG:HH22	6:B:602:DHE:CBB	2.21	0.53
1:B:381:TYR:CD1	1:B:413:VAL:HG22	2.44	0.53
1:B:299:LYS:NZ	1:B:327:HIS:HD2	2.06	0.52
1:B:72:GLY:O	1:B:76:LEU:HG	2.10	0.52
1:B:250:PHE:CD1	1:B:250:PHE:C	2.83	0.52
1:B:36:PHE:HZ	1:B:114:PRO:HG3	1.75	0.51
1:B:378:HIS:CG	1:B:379:PRO:HD2	2.46	0.51
1:B:51:HIS:O	1:B:55:ARG:HA	2.11	0.51
5:B:601:HEC:HBC3	5:B:601:HEC:HMC1	1.92	0.51
1:A:181:VAL:HA	1:A:197:GLY:HA2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:LYS:HD2	1:B:392:ASP:OD2	2.10	0.51
1:B:426:ILE:HG13	1:B:437:VAL:HG22	1.93	0.51
1:B:56:LYS:HE2	7:B:1003:HOH:O	2.10	0.51
1:B:405:HIS:N	1:B:406:PRO:HD3	2.26	0.50
1:A:439:THR:OG1	1:A:442:ASN:HB2	2.11	0.50
1:A:6:ALA:HB1	1:B:422:GLY:HA2	1.94	0.50
1:A:270:THR:O	1:A:274:GLN:HA	2.11	0.50
1:A:306:LEU:HB2	1:A:318:THR:HB	1.94	0.50
1:B:148:PRO:HB2	1:B:488:LYS:HE2	1.94	0.50
1:B:147:LEU:HB2	1:B:148:PRO:HD3	1.95	0.49
1:A:209:ALA:O	1:A:210:LYS:C	2.51	0.49
1:A:381:TYR:CD2	1:A:413:VAL:HG13	2.48	0.49
1:A:114:PRO:HB2	1:B:22:VAL:CG1	2.39	0.48
1:A:267:ARG:NH1	7:A:1040:HOH:O	2.44	0.48
1:B:55:ARG:HB3	1:B:63:LEU:HB2	1.94	0.48
1:B:386:SER:HB3	1:B:397:LEU:HD23	1.95	0.48
1:A:298:VAL:HG12	1:A:301:THR:OG1	2.14	0.48
1:A:188:ALA:HB3	1:A:236:GLU:HG2	1.95	0.48
1:B:334:SER:O	1:B:335:HIS:HB2	2.13	0.48
1:A:10:TYR:OH	1:B:327:HIS:CE1	2.64	0.48
1:B:299:LYS:HZ1	1:B:327:HIS:HD2	1.62	0.47
1:B:436:TYR:CE1	1:B:493:VAL:HG21	2.49	0.47
1:B:250:PHE:CD1	1:B:250:PHE:O	2.68	0.47
1:B:181:VAL:HA	1:B:197:GLY:HA2	1.95	0.47
1:A:343:ASN:OD1	1:A:344:ASN:N	2.43	0.47
1:A:378:HIS:CG	1:A:379:PRO:HD2	2.49	0.47
1:A:424:LEU:HB3	1:A:425:PHE:CD2	2.49	0.47
1:B:370:PRO:HB3	1:B:387:THR:HB	1.97	0.47
1:A:145:LEU:HD11	1:A:172:VAL:HG11	1.97	0.47
1:A:439:THR:HG23	1:A:447:ILE:O	2.15	0.47
1:B:79:LEU:HD13	5:B:601:HEC:HAA1	1.97	0.47
1:B:381:TYR:CD1	1:B:413:VAL:CG2	2.99	0.46
1:B:279:GLU:N	1:B:280:PRO:HD3	2.30	0.46
1:A:198:ARG:NH2	6:A:602:DHE:O2B	2.47	0.46
1:A:219:LYS:HE2	7:A:857:HOH:O	2.16	0.46
1:A:250:PHE:C	1:A:250:PHE:CD1	2.89	0.46
1:A:160:GLN:NE2	7:A:1031:HOH:O	2.49	0.46
1:B:378:HIS:ND1	1:B:379:PRO:HD2	2.30	0.46
1:A:223:GLU:HG2	1:A:245:TYR:HB2	1.97	0.46
1:B:267:ARG:NH1	7:B:787:HOH:O	2.46	0.46
1:A:154:THR:O	1:A:529:PRO:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:TYR:CZ	6:B:602:DHE:HGB2	2.51	0.45
1:A:331:TRP:HB3	1:A:335:HIS:HA	1.99	0.45
1:B:331:TRP:HB3	1:B:335:HIS:HA	1.98	0.45
1:B:364:VAL:HG23	1:B:368:PRO:HG3	1.97	0.45
1:A:218:ILE:HD11	1:A:260:PRO:HG3	1.98	0.45
1:A:449:GLN:HB3	1:A:469:ALA:HB3	1.99	0.45
1:A:299:LYS:NZ	1:A:327:HIS:HD2	2.14	0.45
1:A:138:PRO:HB3	1:A:142:LEU:HD11	1.99	0.44
1:A:401:ASP:OD2	1:A:404:ASN:HB2	2.18	0.44
1:B:198:ARG:NH2	6:B:602:DHE:O2B	2.50	0.44
1:A:299:LYS:HB3	1:A:300:GLU:OE1	2.18	0.44
1:A:468:ILE:HB	1:A:481:VAL:HG21	1.99	0.44
1:A:239:TYR:CE1	1:A:312:ILE:HD12	2.52	0.44
6:A:602:DHE:C2C	6:A:602:DHE:O2C	2.65	0.44
1:B:43:TYR:OH	1:B:55:ARG:HG2	2.18	0.44
1:A:44:PHE:HA	1:A:48:ALA:HB2	1.99	0.44
1:A:359:SER:O	1:A:360:ALA:HB2	2.17	0.44
1:B:113:PRO:HA	1:B:114:PRO:HD3	1.90	0.44
1:B:218:ILE:HD11	1:B:260:PRO:HG3	1.99	0.44
1:A:223:GLU:O	1:A:245:TYR:N	2.51	0.44
1:B:299:LYS:HB3	1:B:300:GLU:OE1	2.18	0.44
1:A:334:SER:O	1:A:335:HIS:HB2	2.18	0.44
1:A:243:GLY:HA3	1:A:282:VAL:HG11	1.99	0.43
1:A:453:VAL:HG21	1:A:466:LEU:HD22	2.00	0.43
1:A:281:ARG:HD2	1:A:300:GLU:OE2	2.19	0.43
1:A:99:LYS:HE2	1:A:102:ILE:HD12	2.00	0.43
1:A:156:ARG:HB3	1:A:157:ASP:H	1.62	0.43
1:A:381:TYR:HB3	1:A:413:VAL:HG21	2.01	0.43
1:A:279:GLU:N	1:A:280:PRO:HD3	2.32	0.43
1:B:33:GLU:HG2	1:B:37:ASN:ND2	2.34	0.43
1:B:436:TYR:CZ	1:B:493:VAL:HG21	2.54	0.43
1:A:279:GLU:N	1:A:280:PRO:CD	2.82	0.42
1:A:336:ARG:NH1	1:A:354:LYS:HB3	2.34	0.42
1:B:115:GLN:HA	1:B:116:PRO:HD3	1.90	0.42
1:A:81:THR:HG23	1:A:92:GLY:HA3	2.00	0.42
1:B:90:ASN:HD22	1:B:93:SER:HB2	1.84	0.42
1:B:403:LYS:HG3	7:B:822:HOH:O	2.19	0.42
1:A:280:PRO:HB3	1:A:301:THR:HG23	2.01	0.42
1:B:79:LEU:HD13	5:B:601:HEC:CAA	2.50	0.42
1:B:149:ASN:HB2	1:B:488:LYS:HE3	2.01	0.42
1:B:405:HIS:N	1:B:406:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLN:HA	1:A:116:PRO:HD3	1.90	0.42
1:A:143:ASN:OD1	1:A:145:LEU:HB2	2.20	0.42
1:B:154:THR:O	1:B:529:PRO:HA	2.19	0.42
1:A:56:LYS:HG2	1:A:62:PRO:HB3	2.01	0.41
1:B:338:PHE:HB3	1:B:351:ILE:HB	2.01	0.41
1:B:487:ASN:HD21	1:B:489:ARG:CG	2.31	0.41
1:A:188:ALA:CB	1:A:236:GLU:HG2	2.50	0.41
1:B:381:TYR:CG	1:B:413:VAL:HG21	2.55	0.41
1:A:299:LYS:HZ1	1:A:327:HIS:CD2	2.38	0.41
1:A:336:ARG:HH11	1:A:354:LYS:HB3	1.85	0.41
1:A:198:ARG:HH22	6:A:602:DHE:CBB	2.34	0.41
1:A:327:HIS:CE1	1:B:10:TYR:OH	2.70	0.41
1:A:403:LYS:HB2	1:A:403:LYS:NZ	2.35	0.41
1:B:121:MET:SD	1:B:260:PRO:HB2	2.61	0.41
1:A:65:PRO:HA	1:A:68:THR:OG1	2.21	0.41
1:A:121:MET:SD	1:A:260:PRO:HB2	2.61	0.41
1:B:247:PRO:O	1:B:249:GLN:HG2	2.21	0.41
1:B:156:ARG:HB3	1:B:157:ASP:H	1.79	0.41
1:A:228:GLU:CG	1:A:229:SER:N	2.83	0.40
1:A:364:VAL:HB	1:A:365:GLY:H	1.69	0.40
1:B:481:VAL:HA	1:B:496:SER:O	2.22	0.40

All (5) 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)
1:B:70:GLN:NE2	1:B:473:ASP:O[3_556]	1.93	0.27
7:A:616:HOH:O	7:A:772:HOH:O[3_545]	2.01	0.19
7:B:706:HOH:O	7:B:874:HOH:O[3_546]	2.07	0.13
1:B:74:GLN:OE1	1:B:169:LYS:O[3_556]	2.08	0.12
7:B:768:HOH:O	7:B:898:HOH:O[3_556]	2.18	0.02

## 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	536/543 (99%)	496 (92%)	35 (6%)	5 (1%)	17	11
1	B	537/543 (99%)	502 (94%)	31 (6%)	4 (1%)	22	15
All	All	1073/1086 (99%)	998 (93%)	66 (6%)	9 (1%)	19	12

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	156	ARG
1	A	299	LYS
1	B	156	ARG
1	B	299	LYS
1	B	26	ASN
1	B	483	GLN
1	A	292	PRO
1	A	483	GLN

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	453/458 (99%)	444 (98%)	9 (2%)	55	59
1	B	454/458 (99%)	448 (99%)	6 (1%)	69	74
All	All	907/916 (99%)	892 (98%)	15 (2%)	60	65

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ARG
1	A	79	LEU
1	A	90	ASN
1	A	99	LYS

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Mol	Chain	Res	Type
1	A	193	LEU
1	A	198	ARG
1	A	336	ARG
1	A	413	VAL
1	A	424	LEU
1	B	198	ARG
1	B	407	GLN
1	B	413	VAL
1	B	424	LEU
1	B	439	THR
1	B	489	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	111	HIS
1	A	115	GLN
1	A	160	GLN
1	A	274	GLN
1	A	327	HIS
1	A	344	ASN
1	B	73	GLN
1	B	90	ASN
1	B	110	GLN
1	B	115	GLN
1	B	160	GLN
1	B	289	HIS
1	B	314	ASN
1	B	327	HIS
1	B	344	ASN

### 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](#)

Of 10 ligands modelled in this entry, 2 are monoatomic and 2 are modelled with single atom - leaving 6 for Mogul analysis.

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	PO4	B	604	-	4,4,4	3.25	4 (100%)	6,6,6	1.18	0
2	PO4	A	604	-	4,4,4	3.29	4 (100%)	6,6,6	0.55	0
5	HEC	A	601	1	32,50,50	1.77	3 (9%)	24,82,82	1.43	3 (12%)
6	DHE	A	602	1,4	50,56,56	1.64	7 (14%)	44,94,94	2.24	9 (20%)
6	DHE	B	602	1,4	50,56,56	1.65	7 (14%)	44,94,94	2.32	10 (22%)
5	HEC	B	601	1	32,50,50	1.50	2 (6%)	24,82,82	0.96	1 (4%)

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
6	DHE	B	602	1,4	1/1/15/19	8/20/108/108	-
5	HEC	A	601	1	-	2/10/54/54	-
5	HEC	B	601	1	-	2/10/54/54	-
6	DHE	A	602	1,4	1/1/15/19	6/20/108/108	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	HEC	C3C-C2C	-5.97	1.34	1.40
5	A	601	HEC	C2B-C3B	-5.36	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	604	PO4	P-O1	4.98	1.62	1.50
6	A	602	DHE	CAD-CBD	-4.68	1.29	1.52
6	B	602	DHE	CAD-CBD	-4.63	1.29	1.52
2	B	604	PO4	P-O1	4.53	1.61	1.50
5	B	601	HEC	C2B-C3B	-4.40	1.36	1.40
5	B	601	HEC	C3C-C2C	-4.16	1.36	1.40
6	B	602	DHE	CGC-C3C	4.14	1.62	1.54
6	A	602	DHE	CGB-C3B	4.04	1.61	1.54
6	A	602	DHE	CGC-C3C	3.78	1.61	1.54
6	B	602	DHE	CGB-C3B	3.73	1.61	1.54
6	B	602	DHE	CHA-C1A	3.57	1.40	1.35
6	B	602	DHE	CAD-C3D	-3.37	1.47	1.52
6	A	602	DHE	CAD-C3D	-3.32	1.47	1.52
6	A	602	DHE	FE-NA	3.04	2.07	1.95
6	B	602	DHE	FE-NA	2.95	2.07	1.95
6	A	602	DHE	CHA-C1A	2.90	1.39	1.35
2	B	604	PO4	P-O3	2.81	1.63	1.54
2	B	604	PO4	P-O2	2.79	1.63	1.54
2	A	604	PO4	P-O4	2.72	1.62	1.54
5	A	601	HEC	C1D-ND	2.71	1.41	1.36
2	B	604	PO4	P-O4	2.45	1.62	1.54
2	A	604	PO4	P-O3	2.45	1.62	1.54
2	A	604	PO4	P-O2	2.25	1.61	1.54
6	A	602	DHE	FE-NC	2.14	2.08	1.97
6	B	602	DHE	FE-NC	2.01	2.08	1.97

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	602	DHE	CBD-CAD-C3D	8.46	127.06	112.62
6	A	602	DHE	CBD-CAD-C3D	7.59	125.58	112.62
6	B	602	DHE	C1C-NC-C4C	5.72	110.98	105.07
6	A	602	DHE	C1C-NC-C4C	5.65	110.91	105.07
6	A	602	DHE	C4B-NB-C1B	5.44	110.69	105.07
6	B	602	DHE	C4B-NB-C1B	5.29	110.53	105.07
6	A	602	DHE	CAD-CBD-CGD	4.75	127.07	113.76
6	B	602	DHE	CAD-CBD-CGD	4.34	125.93	113.76
6	B	602	DHE	C4A-NA-C1A	3.87	109.13	105.35
5	A	601	HEC	CBD-CAD-C3D	-3.47	106.70	112.62
6	A	602	DHE	C4A-NA-C1A	3.21	108.49	105.35
6	A	602	DHE	CHB-C1B-NB	3.03	127.71	124.42
5	A	601	HEC	C1D-C2D-C3D	-2.92	104.97	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	602	DHE	CMD-C2D-C1D	-2.88	124.04	128.46
6	B	602	DHE	C1C-CHC-C4B	2.53	128.83	124.98
6	A	602	DHE	CMD-C2D-C1D	-2.45	124.70	128.46
6	A	602	DHE	C1C-CHC-C4B	2.42	128.67	124.98
6	A	602	DHE	CHC-C1C-NC	2.35	126.97	124.42
6	B	602	DHE	CHB-C1B-NB	2.29	126.91	124.42
6	B	602	DHE	CHC-C1C-NC	2.25	126.86	124.42
6	B	602	DHE	C2A-C1A-NA	-2.18	108.20	110.32
5	A	601	HEC	CMB-C2B-C3B	2.07	128.25	125.82
5	B	601	HEC	CBA-CAA-C2A	2.01	115.99	112.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	602	DHE	NA
6	B	602	DHE	NA

All (18) torsion outliers are listed below:

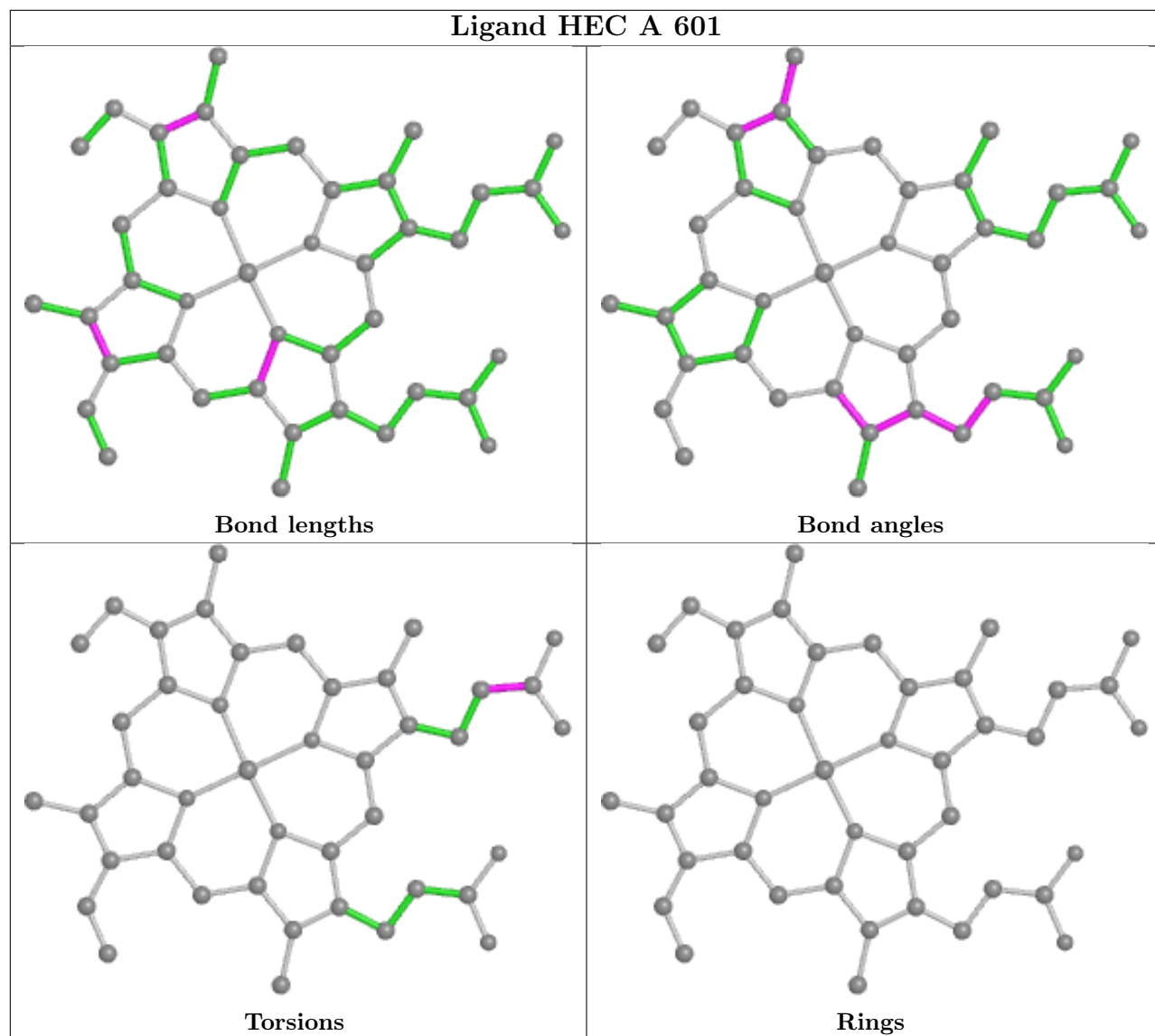
Mol	Chain	Res	Type	Atoms
6	A	602	DHE	C2D-C3D-CAD-CBD
6	A	602	DHE	C4D-C3D-CAD-CBD
6	B	602	DHE	C2D-C3D-CAD-CBD
6	B	602	DHE	C4D-C3D-CAD-CBD
6	A	602	DHE	C3C-CAC-CBC-O1C
6	A	602	DHE	C3B-CAB-CBB-O1B
6	B	602	DHE	C3B-CAB-CBB-O1B
6	B	602	DHE	C3C-CAC-CBC-O1C
6	B	602	DHE	C3C-CAC-CBC-O2C
6	A	602	DHE	C3B-CAB-CBB-O2B
6	A	602	DHE	C3C-CAC-CBC-O2C
6	B	602	DHE	C3B-CAB-CBB-O2B
5	B	601	HEC	CAA-CBA-CGA-O1A
5	B	601	HEC	CAA-CBA-CGA-O2A
5	A	601	HEC	CAA-CBA-CGA-O2A
5	A	601	HEC	CAA-CBA-CGA-O1A
6	B	602	DHE	CAA-CBA-CGA-O2A
6	B	602	DHE	CAA-CBA-CGA-O1A

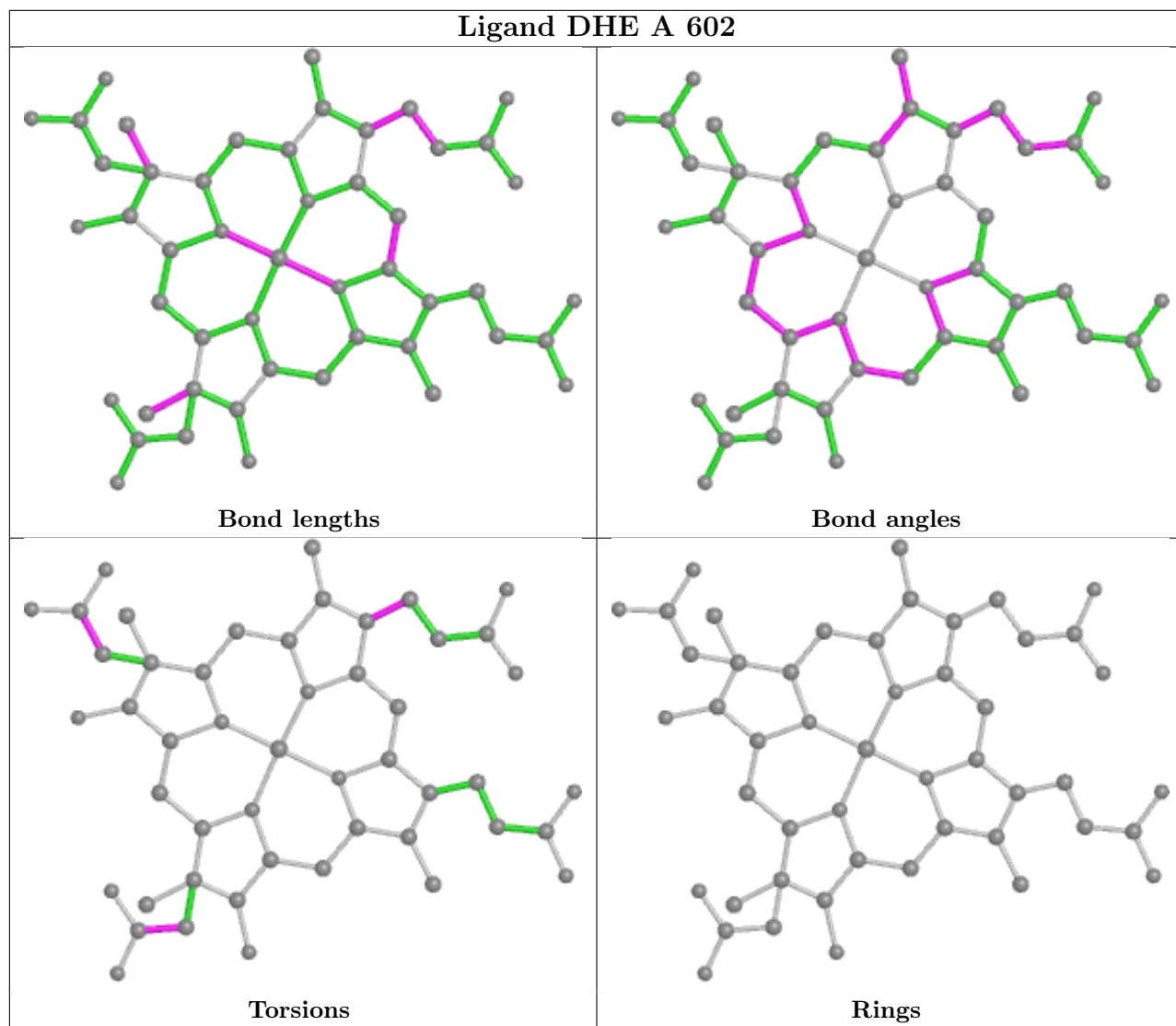
There are no ring outliers.

4 monomers are involved in 10 short contacts:

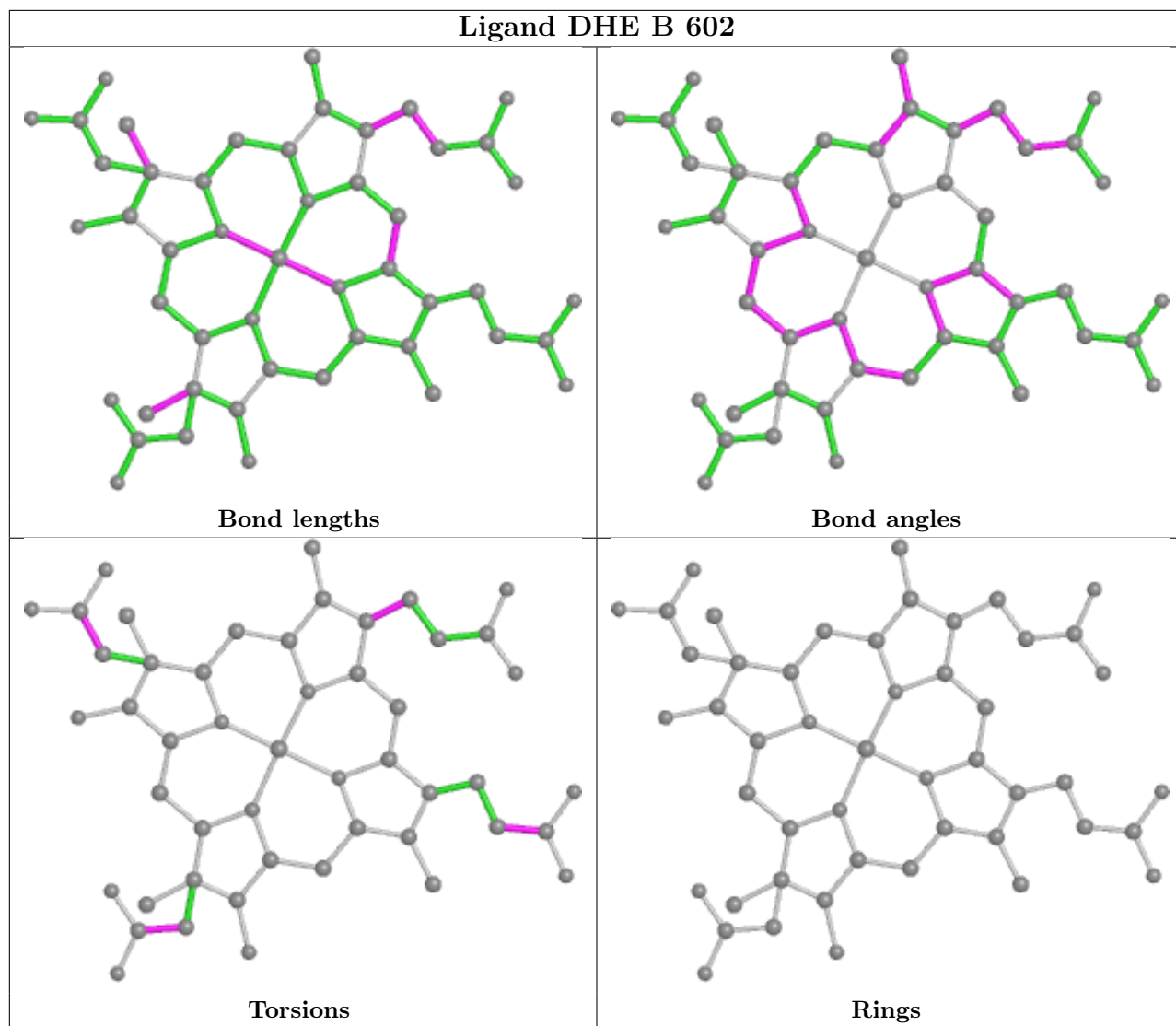
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	HEC	1	0
6	A	602	DHE	3	0
6	B	602	DHE	3	0
5	B	601	HEC	3	0

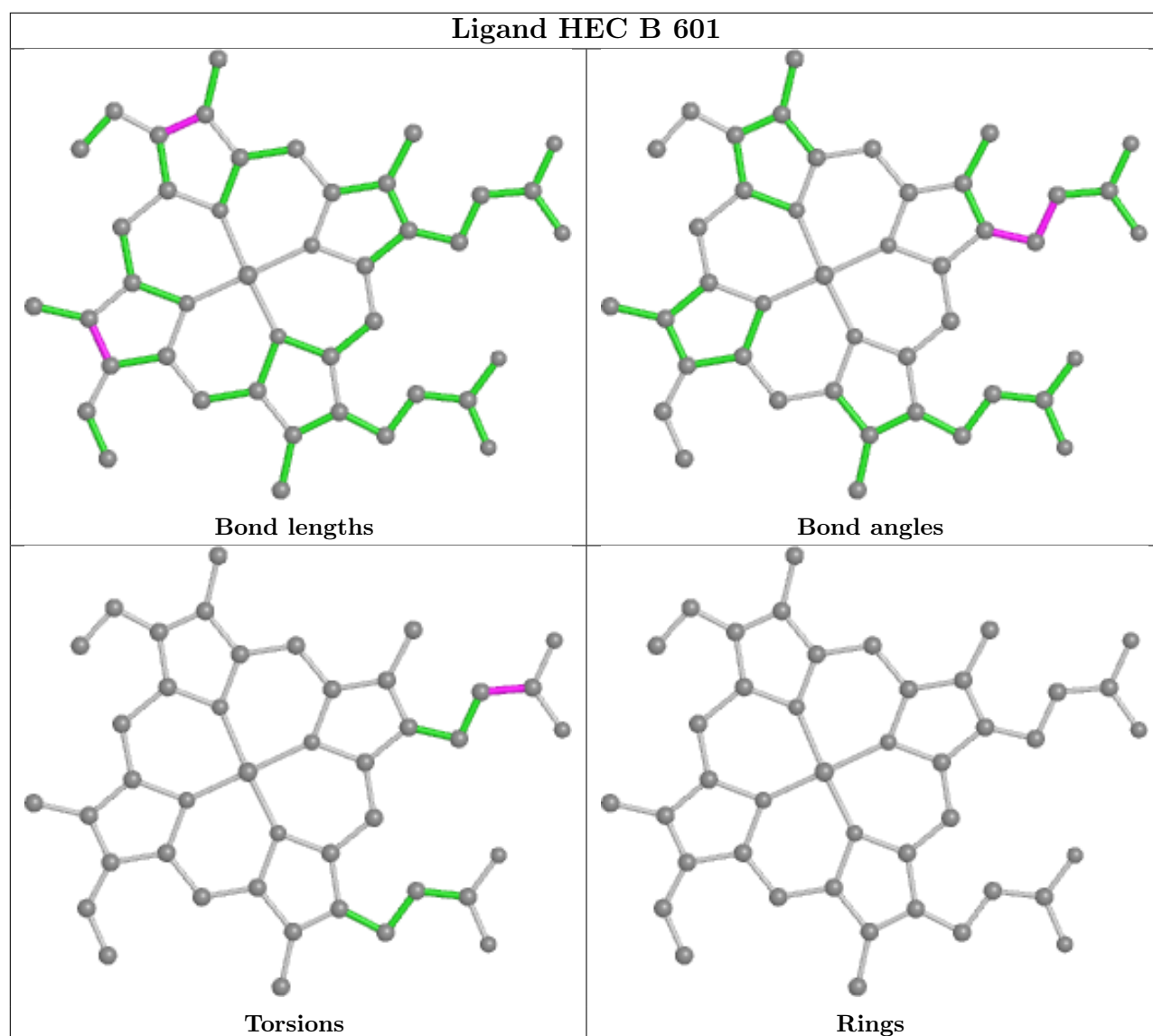
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	248:PRO	C	249:GLN	N	1.19

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

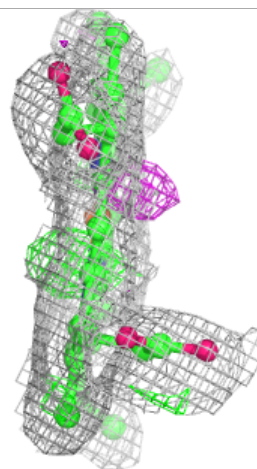
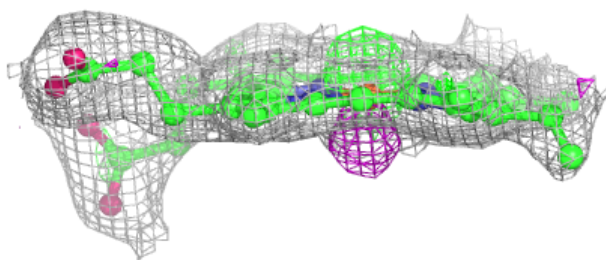
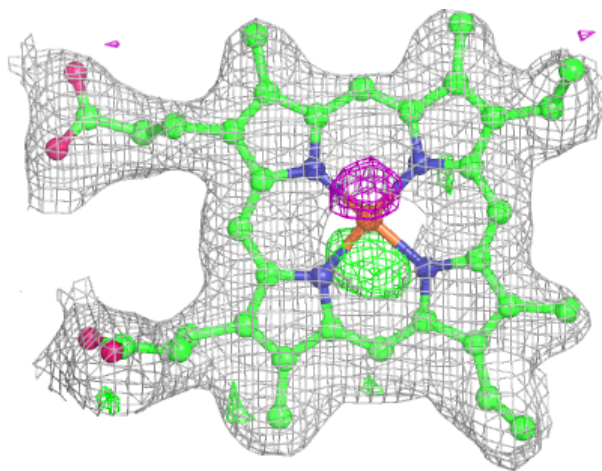
### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

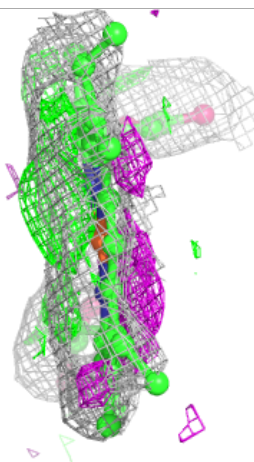
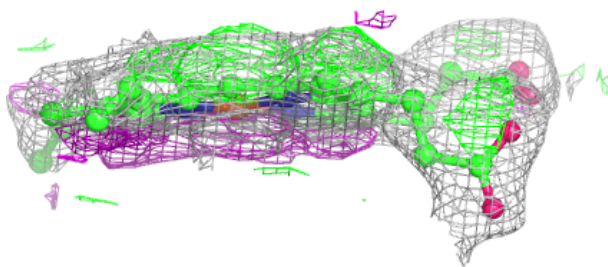
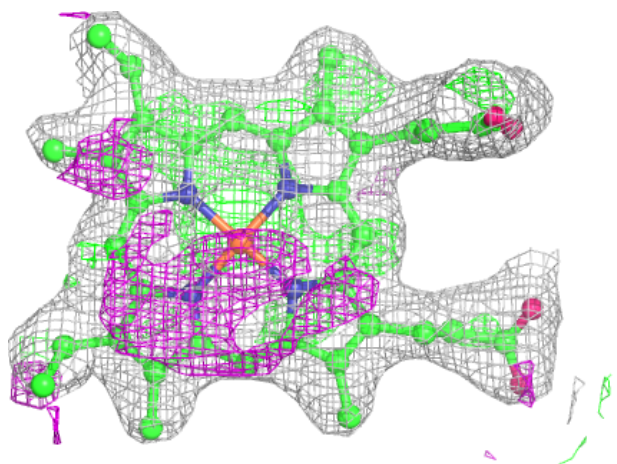
**Electron density around HEC A 601:**

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



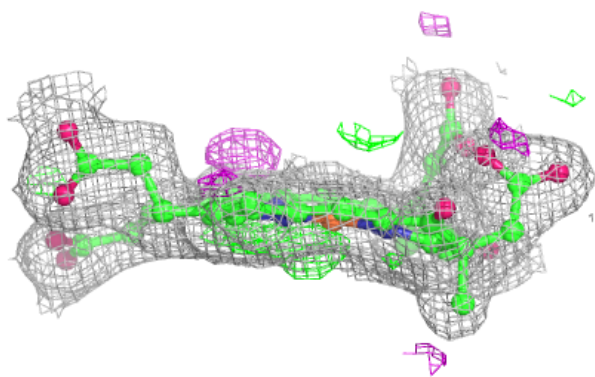
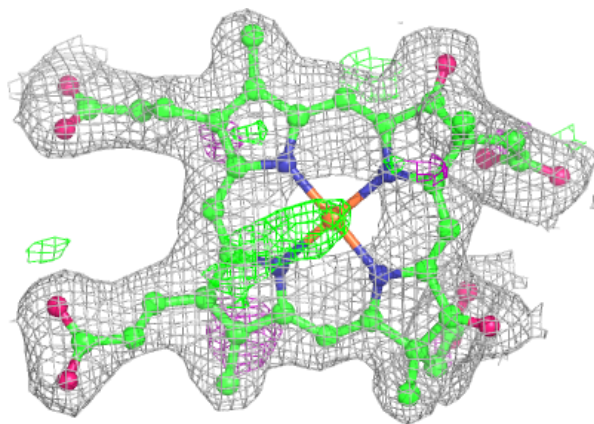
**Electron density around HEC B 601:**

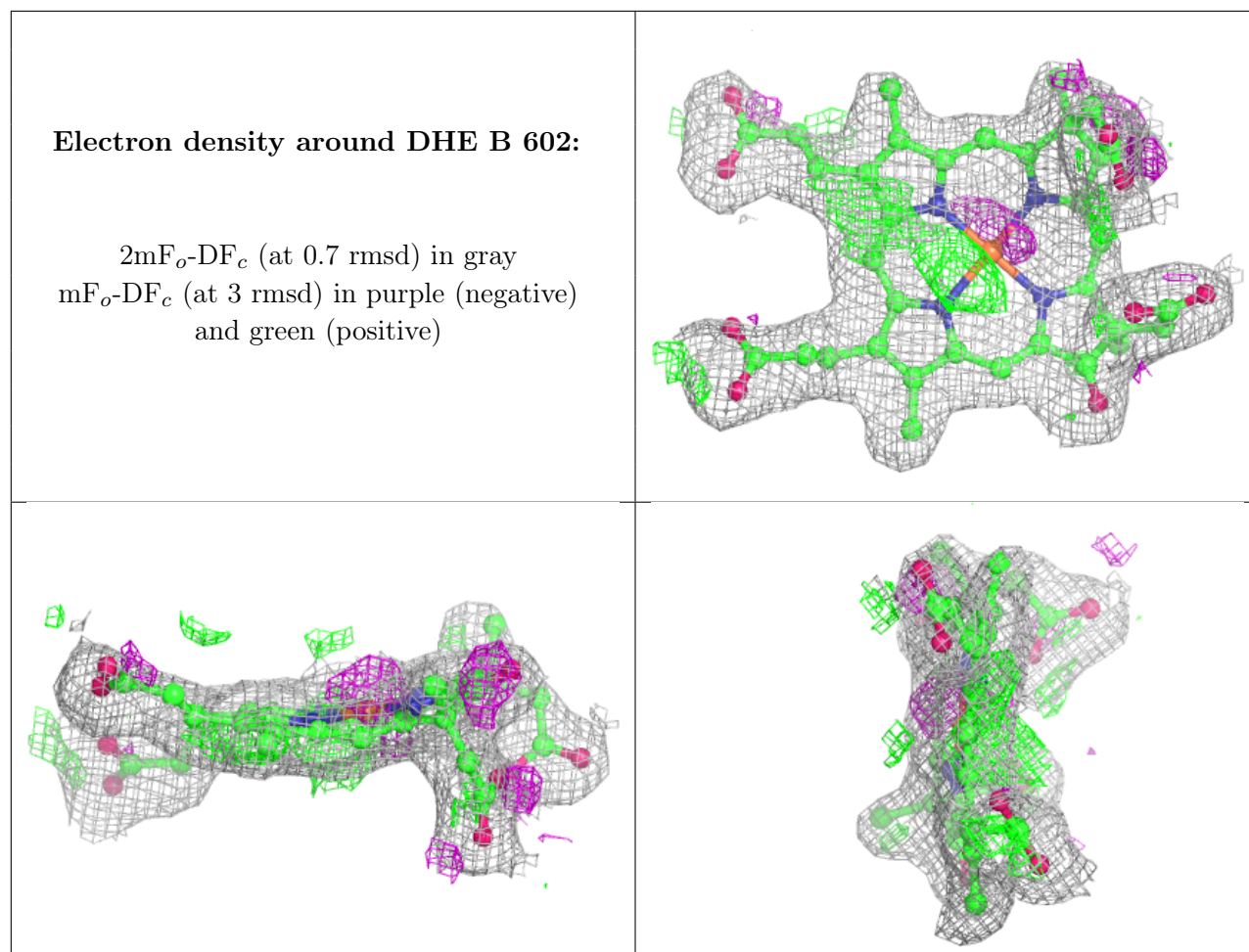
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around DHE A 602:**

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





## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.