



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:56 PM UTC

PDB ID : 1HZV / pdb_00001hzv
Title : DOMAIN SWING UPON HIS TO ALA MUTATION IN NITRITE REDUCTASE OF PSEUDOMONAS AERUGINOSA
Authors : Brown, K.; Tegoni, M.; Cambillau, C.
Deposited on : 2001-01-26
Resolution : 2.83 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

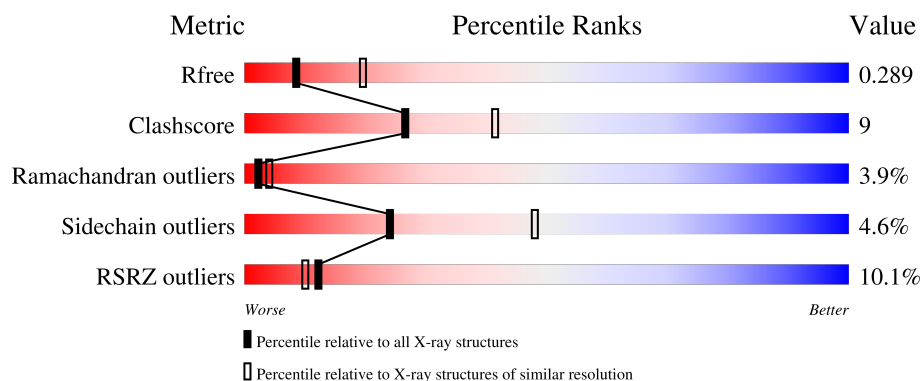
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	543	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4456 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.

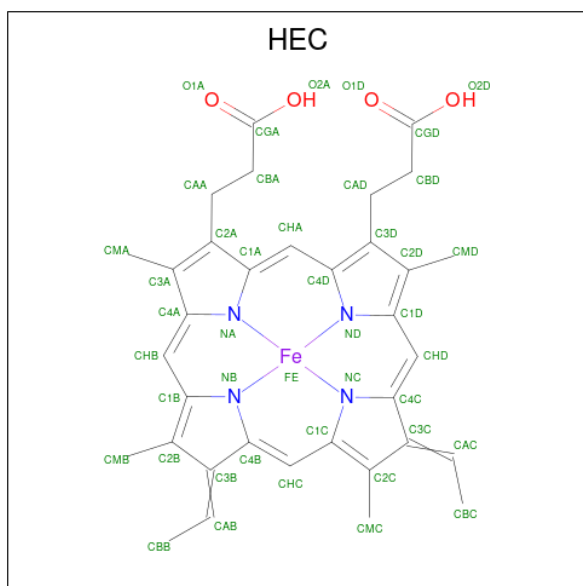
- Molecule 1 is a protein called NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4032	2560	701	759	12			

There is a discrepancy between the modelled and reference sequences:

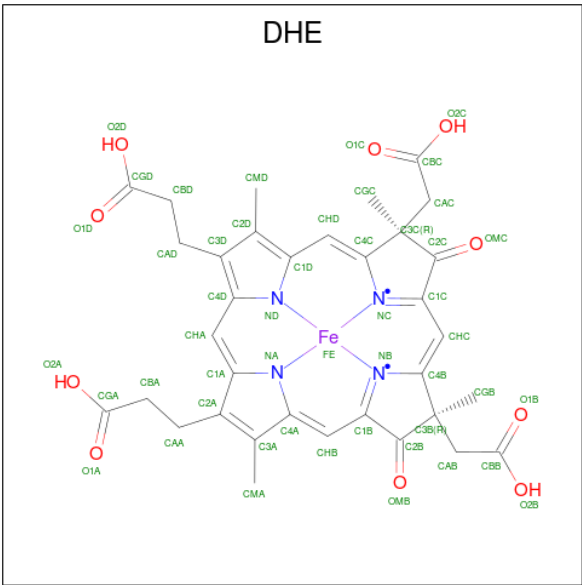
Chain	Residue	Modelled	Actual	Comment	Reference
A	369	ALA	HIS	engineered mutation	UNP P24474

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



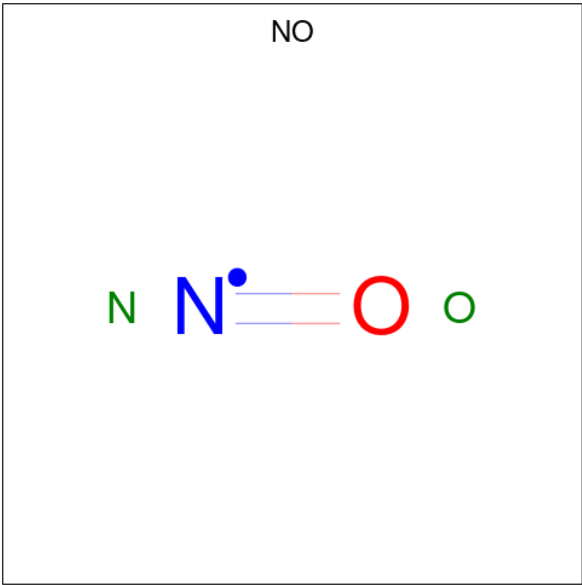
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 3 is HEME D (CCD ID: DHE) (formula: $C_{34}H_{32}FeN_4O_{10}$).



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

- Molecule 4 is NITRIC OXIDE (CCD ID: NO) (formula: NO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			2	1	1		

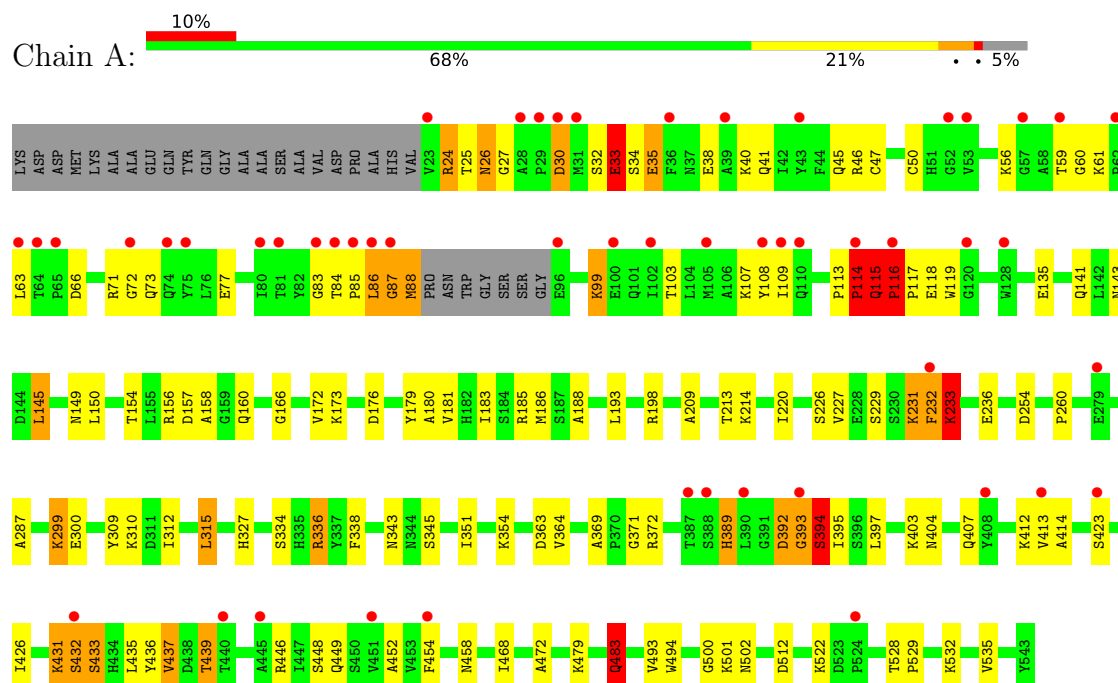
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	330	Total 330	O 330	0	0

3 Residue-property plots [i](#)

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

• Molecule 1: NITRITE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	94.74Å 94.74Å 159.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.83 19.91 – 2.83	Depositor EDS
% Data completeness (in resolution range)	96.6 (19.91-2.83) 96.3 (19.91-2.83)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.88 (at 2.85Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.282 , 0.296 0.280 , 0.289	Depositor DCC
R_{free} test set	436 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å ²)	81.5	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4456	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: NO, DHE, HEC

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	0.96	10/4129 (0.2%)	1.40	63/5604 (1.1%)

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	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	433	SER	C-O	11.94	1.39	1.24
1	A	33	GLU	CA-C	-10.74	1.38	1.52
1	A	32	SER	C-O	10.66	1.37	1.23
1	A	426	ILE	CB-CG2	-7.00	1.29	1.52
1	A	86	LEU	CG-CD1	-6.66	1.30	1.52
1	A	393	GLY	C-O	6.17	1.33	1.24
1	A	494	TRP	NE1-CE2	-5.92	1.30	1.37
1	A	50	CYS	CB-SG	5.77	2.00	1.81
1	A	260	PRO	CA-CB	-5.30	1.46	1.53
1	A	432	SER	N-CA	-5.26	1.40	1.46

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	371	GLY	N-CA-C	-12.22	96.69	111.35
1	A	32	SER	N-CA-C	11.80	128.43	110.14
1	A	432	SER	CA-C-N	11.29	143.11	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	SER	C-N-CA	11.29	143.11	121.54
1	A	433	SER	N-CA-C	10.89	134.00	110.80
1	A	393	GLY	N-CA-C	-10.82	92.74	111.57
1	A	118	GLU	N-CA-C	10.21	125.28	113.02
1	A	114	PRO	N-CA-C	9.56	124.60	111.22
1	A	343	ASN	N-CA-C	9.36	122.35	111.11
1	A	432	SER	N-CA-C	9.33	122.55	108.46
1	A	32	SER	O-C-N	9.17	134.93	123.10
1	A	433	SER	CA-C-O	-8.64	108.16	120.51
1	A	109	ILE	N-CA-C	-8.46	102.82	113.22
1	A	432	SER	O-C-N	8.35	132.71	123.52
1	A	24	ARG	N-CA-C	7.82	122.30	109.24
1	A	431	LYS	N-CA-C	7.48	121.66	112.23
1	A	33	GLU	CA-C-O	-7.39	109.95	120.51
1	A	108	TYR	N-CA-C	7.37	122.45	113.17
1	A	116	PRO	N-CA-C	7.17	119.45	110.70
1	A	85	PRO	N-CA-C	7.08	122.04	114.68
1	A	72	GLY	N-CA-C	6.83	121.34	112.18
1	A	433	SER	CA-C-N	-6.82	111.90	122.87
1	A	433	SER	C-N-CA	-6.82	111.90	122.87
1	A	26	ASN	N-CA-C	6.81	121.04	113.21
1	A	60	GLY	N-CA-C	-6.70	101.36	111.14
1	A	88	MET	N-CA-C	-6.61	92.50	111.00
1	A	61	LYS	CA-C-N	6.53	128.00	119.84
1	A	61	LYS	C-N-CA	6.53	128.00	119.84
1	A	232	PHE	CA-C-N	6.43	133.82	121.54
1	A	232	PHE	C-N-CA	6.43	133.82	121.54
1	A	300	GLU	N-CA-C	6.21	118.85	111.33
1	A	483	GLN	N-CA-C	6.20	123.52	109.81
1	A	220	ILE	N-CA-C	6.15	118.92	112.83
1	A	231	LYS	N-CA-C	6.01	120.22	112.41
1	A	41	GLN	N-CA-C	-5.93	105.53	112.89
1	A	413	VAL	N-CA-C	5.90	116.03	110.30
1	A	334	SER	N-CA-C	5.89	120.33	113.20
1	A	30	ASP	CA-C-N	5.85	131.95	122.29
1	A	30	ASP	C-N-CA	5.85	131.95	122.29
1	A	114	PRO	CA-C-N	5.75	135.82	121.80
1	A	114	PRO	C-N-CA	5.75	135.82	121.80
1	A	432	SER	N-CA-CB	5.71	120.25	110.77
1	A	115	GLN	CA-C-N	5.70	126.25	120.38
1	A	115	GLN	C-N-CA	5.70	126.25	120.38
1	A	33	GLU	O-C-N	5.63	130.07	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	392	ASP	N-CA-C	-5.61	101.87	109.95
1	A	116	PRO	CA-C-N	5.57	125.57	119.89
1	A	116	PRO	C-N-CA	5.57	125.57	119.89
1	A	226	SER	N-CA-C	5.56	118.79	109.95
1	A	113	PRO	CA-C-N	5.47	125.47	120.21
1	A	113	PRO	C-N-CA	5.47	125.47	120.21
1	A	141	GLN	N-CA-C	5.40	117.85	110.24
1	A	115	GLN	N-CA-C	5.40	121.73	109.81
1	A	389	HIS	N-CA-C	5.35	118.00	109.81
1	A	315	LEU	N-CA-C	5.33	118.63	110.20
1	A	433	SER	O-C-N	5.25	129.57	122.59
1	A	394	SER	N-CA-C	-5.18	99.76	110.80
1	A	233	LYS	CB-CG-CD	5.08	122.98	111.30
1	A	38	GLU	N-CA-C	5.08	117.93	111.69
1	A	309	TYR	N-CA-C	5.08	119.62	113.38
1	A	394	SER	N-CA-CB	5.07	119.06	110.49
1	A	145	LEU	N-CA-C	5.04	117.61	110.10
1	A	312	ILE	N-CA-C	5.02	118.17	111.44

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	PRO	Mainchain
1	A	33	GLU	Mainchain
1	A	87	GLY	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4032	0	4011	72	0
2	A	43	0	30	3	0
3	A	49	0	24	3	0
4	A	2	0	0	0	0
5	A	330	0	0	11	0
All	All	4456	0	4065	74	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 9.

All (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:MET:HE1	5:A:782:HOH:O	1.51	1.10
1:A:299:LYS:HZ1	1:A:327:HIS:CD2	1.75	1.03
1:A:40:LYS:HD2	1:A:114:PRO:HB3	1.51	0.92
1:A:25:THR:HG22	1:A:26:ASN:H	1.37	0.90
1:A:157:ASP:OD1	5:A:906:HOH:O	1.92	0.86
3:A:602:DHE:HH1	5:A:878:HOH:O	1.74	0.85
1:A:46:ARG:HH22	1:A:179:TYR:HB2	1.44	0.81
1:A:299:LYS:NZ	1:A:327:HIS:CD2	2.53	0.77
1:A:231:LYS:HE2	5:A:890:HOH:O	1.85	0.76
1:A:114:PRO:O	1:A:116:PRO:HD3	1.88	0.74
1:A:232:PHE:CE1	1:A:233:LYS:HG2	2.23	0.74
1:A:299:LYS:HZ1	1:A:327:HIS:HD2	1.34	0.72
1:A:33:GLU:O	1:A:35:GLU:N	2.23	0.71
1:A:40:LYS:HD2	1:A:114:PRO:CB	2.22	0.70
1:A:299:LYS:NZ	1:A:327:HIS:HD2	1.88	0.69
1:A:84:THR:OG1	2:A:601:HEC:O1D	2.10	0.69
1:A:299:LYS:HZ1	1:A:327:HIS:CG	2.14	0.66
1:A:395:ILE:HD11	1:A:437:VAL:HG11	1.80	0.64
1:A:83:GLY:HA2	1:A:88:MET:HG3	1.82	0.62
1:A:145:LEU:HD21	1:A:172:VAL:HG11	1.80	0.62
1:A:83:GLY:CA	1:A:88:MET:HG3	2.31	0.61
1:A:180:ALA:HB3	1:A:198:ARG:HG2	1.82	0.60
1:A:173:LYS:HD2	5:A:849:HOH:O	2.02	0.60
1:A:59:THR:HG21	5:A:667:HOH:O	2.02	0.59
1:A:431:LYS:O	1:A:432:SER:HB3	2.05	0.57
1:A:185:ARG:HD2	1:A:227:VAL:O	2.04	0.56
1:A:336:ARG:HH11	1:A:354:LYS:HB3	1.71	0.56
1:A:24:ARG:HA	1:A:30:ASP:CG	2.32	0.55
1:A:437:VAL:HG22	1:A:452:ALA:HB3	1.88	0.55
1:A:66:ASP:O	1:A:66:ASP:OD1	2.25	0.55
1:A:25:THR:HG22	1:A:26:ASN:N	2.14	0.54
1:A:25:THR:CG2	1:A:26:ASN:H	2.15	0.53
1:A:46:ARG:NH2	1:A:179:TYR:HB2	2.18	0.52
1:A:185:ARG:HH21	3:A:602:DHE:CGA	2.22	0.51
1:A:87:GLY:HA2	1:A:501:LYS:NZ	2.25	0.51
1:A:395:ILE:CD1	1:A:437:VAL:HG11	2.40	0.51
1:A:186:MET:HE2	1:A:535:VAL:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ARG:NH2	5:A:877:HOH:O	2.44	0.50
1:A:46:ARG:HH22	1:A:179:TYR:CB	2.20	0.50
1:A:397:LEU:HD12	1:A:414:ALA:HB3	1.94	0.50
1:A:149:ASN:ND2	1:A:166:GLY:HA3	2.27	0.49
1:A:287:ALA:HB1	5:A:856:HOH:O	2.12	0.49
1:A:392:ASP:HB3	1:A:393:GLY:O	2.12	0.49
1:A:369:ALA:HB1	5:A:870:HOH:O	2.12	0.48
1:A:394:SER:OG	1:A:395:ILE:N	2.46	0.48
1:A:472:ALA:O	1:A:522:LYS:HE3	2.14	0.48
1:A:143:ASN:ND2	1:A:209:ALA:O	2.47	0.48
1:A:59:THR:O	1:A:59:THR:HG22	2.15	0.46
2:A:601:HEC:HBC3	5:A:700:HOH:O	2.15	0.45
1:A:116:PRO:HA	1:A:117:PRO:HD2	1.73	0.45
1:A:213:THR:HG22	1:A:214:LYS:H	1.81	0.45
1:A:158:ALA:HB1	1:A:160:GLN:HE21	1.82	0.44
1:A:103:THR:HG22	1:A:107:LYS:HE3	1.98	0.44
1:A:389:HIS:O	1:A:423:SER:HB3	2.17	0.44
1:A:87:GLY:HA2	1:A:501:LYS:HZ2	1.83	0.44
1:A:449:GLN:OE1	1:A:479:LYS:HE2	2.17	0.44
1:A:183:ILE:CD1	1:A:185:ARG:HE	2.31	0.44
1:A:338:PHE:HB3	1:A:351:ILE:HB	2.00	0.43
1:A:435:LEU:HB3	1:A:454:PHE:HB2	2.00	0.43
1:A:84:THR:OG1	2:A:601:HEC:CGD	2.66	0.43
1:A:528:THR:HG21	5:A:906:HOH:O	2.18	0.43
1:A:403:LYS:HE2	1:A:404:ASN:HD21	1.82	0.43
1:A:232:PHE:CG	1:A:233:LYS:N	2.87	0.43
1:A:432:SER:O	1:A:512:ASP:OD2	2.37	0.43
1:A:439:THR:O	1:A:448:SER:HA	2.19	0.42
1:A:73:GLN:O	1:A:77:GLU:HG3	2.18	0.42
1:A:86:LEU:HD23	1:A:502:ASN:OD1	2.19	0.42
1:A:436:TYR:CZ	1:A:493:VAL:HG21	2.55	0.41
1:A:160:GLN:HG2	1:A:176:ASP:HA	2.02	0.41
1:A:185:ARG:NH2	3:A:602:DHE:CGA	2.84	0.41
1:A:483:GLN:HB3	1:A:532:LYS:NZ	2.36	0.41
1:A:99:LYS:O	1:A:103:THR:OG1	2.38	0.41
1:A:154:THR:O	1:A:529:PRO:HA	2.22	0.40
1:A:364:VAL:HA	1:A:412:LYS:HE2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	510/543 (94%)	446 (88%)	44 (9%)	20 (4%)	2 4

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	56	LYS
1	A	115	GLN
1	A	116	PRO
1	A	188	ALA
1	A	233	LYS
1	A	299	LYS
1	A	394	SER
1	A	433	SER
1	A	119	TRP
1	A	156	ARG
1	A	181	VAL
1	A	458	ASN
1	A	236	GLU
1	A	483	GLN
1	A	27	GLY
1	A	345	SER
1	A	468	ILE
1	A	310	LYS
1	A	500	GLY

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	437/457 (96%)	417 (95%)	20 (5%)	24	48

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLU
1	A	35	GLU
1	A	45	GLN
1	A	47	CYS
1	A	63	LEU
1	A	71	ARG
1	A	99	LYS
1	A	115	GLN
1	A	135	GLU
1	A	150	LEU
1	A	193	LEU
1	A	229	SER
1	A	254	ASP
1	A	315	LEU
1	A	336	ARG
1	A	363	ASP
1	A	407	GLN
1	A	437	VAL
1	A	439	THR
1	A	446	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	143	ASN
1	A	160	GLN
1	A	327	HIS
1	A	344	ASN
1	A	375	ASN
1	A	404	ASN
1	A	407	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 ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NO	A	603	-	0,1,1	-	-	-		
2	HEC	A	601	1	46,50,50	1.94	8 (17%)	58,82,82	2.12	10 (17%)
3	DHE	A	602	1	52,56,56	2.19	13 (25%)	68,94,94	1.93	17 (25%)

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	A	601	1	-	7/14/54/54	-
3	DHE	A	602	1	-	8/20/108/108	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	DHE	CBD-CAD	-7.12	1.27	1.51
2	A	601	HEC	CAB-C3B	6.49	1.56	1.35
2	A	601	HEC	CBC-CAC	6.24	1.72	1.49
3	A	602	DHE	FE-NA	5.24	2.12	1.95
3	A	602	DHE	FE-NB	5.22	2.11	1.94
3	A	602	DHE	FE-NC	4.59	2.09	1.94
3	A	602	DHE	CGB-C3B	4.52	1.62	1.54
3	A	602	DHE	FE-ND	4.51	2.10	1.95
2	A	601	HEC	C3C-C4C	-4.31	1.38	1.46
3	A	602	DHE	CGC-C3C	3.78	1.61	1.54
2	A	601	HEC	CAC-C3C	2.95	1.44	1.35
3	A	602	DHE	C1B-C2B	2.66	1.51	1.47
3	A	602	DHE	CBD-CGD	-2.55	1.44	1.50
3	A	602	DHE	O2D-CGD	-2.38	1.22	1.30
2	A	601	HEC	CHD-C1D	-2.38	1.34	1.39
3	A	602	DHE	CBA-CGA	-2.36	1.45	1.50
2	A	601	HEC	CMD-C2D	2.22	1.55	1.50
2	A	601	HEC	CHA-C1A	2.21	1.42	1.38
3	A	602	DHE	CAC-C3C	-2.09	1.48	1.54
2	A	601	HEC	CHB-C4A	2.08	1.42	1.38
3	A	602	DHE	CHB-C4A	2.07	1.42	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEC	CBC-CAC-C3C	-12.71	102.04	127.43
3	A	602	DHE	CBD-CAD-C3D	5.40	127.47	112.53
3	A	602	DHE	C1C-NC-C4C	4.76	110.84	105.21
3	A	602	DHE	CAD-CBD-CGD	4.46	125.50	113.67
3	A	602	DHE	C3C-C4C-CHD	4.45	126.40	122.44
3	A	602	DHE	C1C-CHC-C4B	4.26	132.00	125.23
3	A	602	DHE	C3B-C4B-CHC	4.15	126.13	122.44
3	A	602	DHE	C4B-NB-C1B	3.93	109.86	105.21
3	A	602	DHE	C2A-C1A-NA	-3.09	107.34	110.32
3	A	602	DHE	C3D-C4D-ND	-3.06	106.76	110.15
2	A	601	HEC	O1D-CGD-CBD	-2.98	113.64	123.09
2	A	601	HEC	CHD-C1D-C2D	-2.95	118.86	127.43
3	A	602	DHE	C2B-C3B-C4B	-2.79	98.87	100.35
3	A	602	DHE	C4D-ND-C1D	2.75	110.30	105.82
3	A	602	DHE	CHA-C1A-C2A	2.59	128.96	124.86
2	A	601	HEC	CBA-CAA-C2A	2.59	119.68	112.53
2	A	601	HEC	O2D-CGD-CBD	2.57	122.13	114.00
2	A	601	HEC	CHD-C4C-C3C	-2.54	120.93	125.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	DHE	CHC-C1C-NC	2.49	127.10	124.42
2	A	601	HEC	CAD-C3D-C4D	2.18	129.19	124.94
2	A	601	HEC	CMB-C2B-C1B	-2.16	122.14	125.42
3	A	602	DHE	C4A-NA-C1A	2.13	109.30	105.82
3	A	602	DHE	O1C-CBC-CAC	-2.13	116.92	122.95
2	A	601	HEC	CBD-CAD-C3D	2.07	118.24	112.53
3	A	602	DHE	CHB-C1B-C2B	2.05	124.51	122.21
3	A	602	DHE	C2D-C1D-ND	-2.01	106.92	110.14
2	A	601	HEC	CMB-C2B-C3B	2.01	131.27	126.55

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	HEC	C2B-C3B-CAB-CBB
2	A	601	HEC	C4B-C3B-CAB-CBB
2	A	601	HEC	C4C-C3C-CAC-CBC
3	A	602	DHE	C3B-CAB-CBB-O2B
3	A	602	DHE	C3B-CAB-CBB-O1B
2	A	601	HEC	C2C-C3C-CAC-CBC
3	A	602	DHE	C3C-CAC-CBC-O1C
3	A	602	DHE	CAD-CBD-CGD-O1D
3	A	602	DHE	CAD-CBD-CGD-O2D
3	A	602	DHE	C3C-CAC-CBC-O2C
2	A	601	HEC	CAA-CBA-CGA-O2A
2	A	601	HEC	CAA-CBA-CGA-O1A
3	A	602	DHE	CAA-CBA-CGA-O2A
3	A	602	DHE	CAA-CBA-CGA-O1A
2	A	601	HEC	CAD-CBD-CGD-O2D

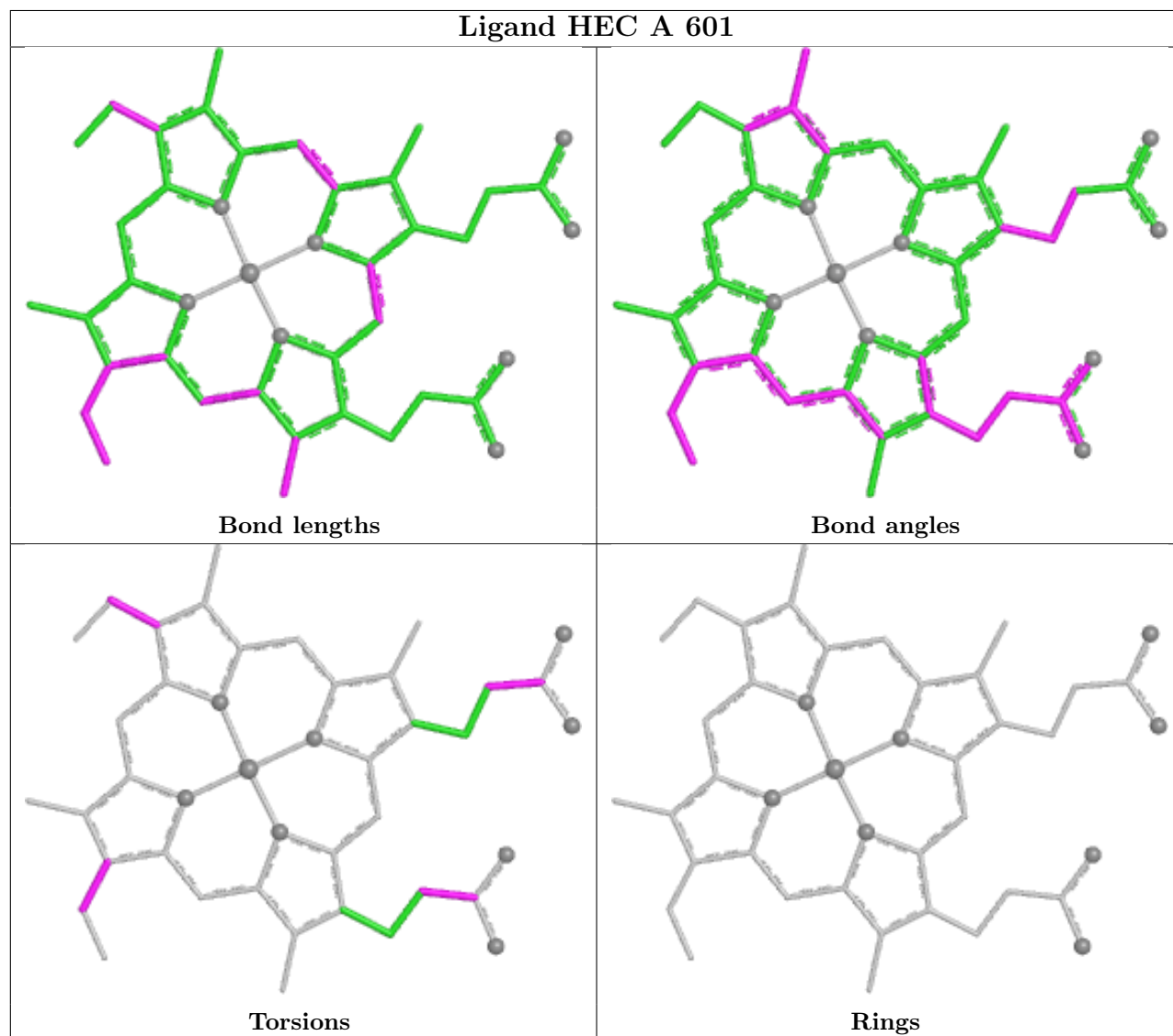
There are no ring outliers.

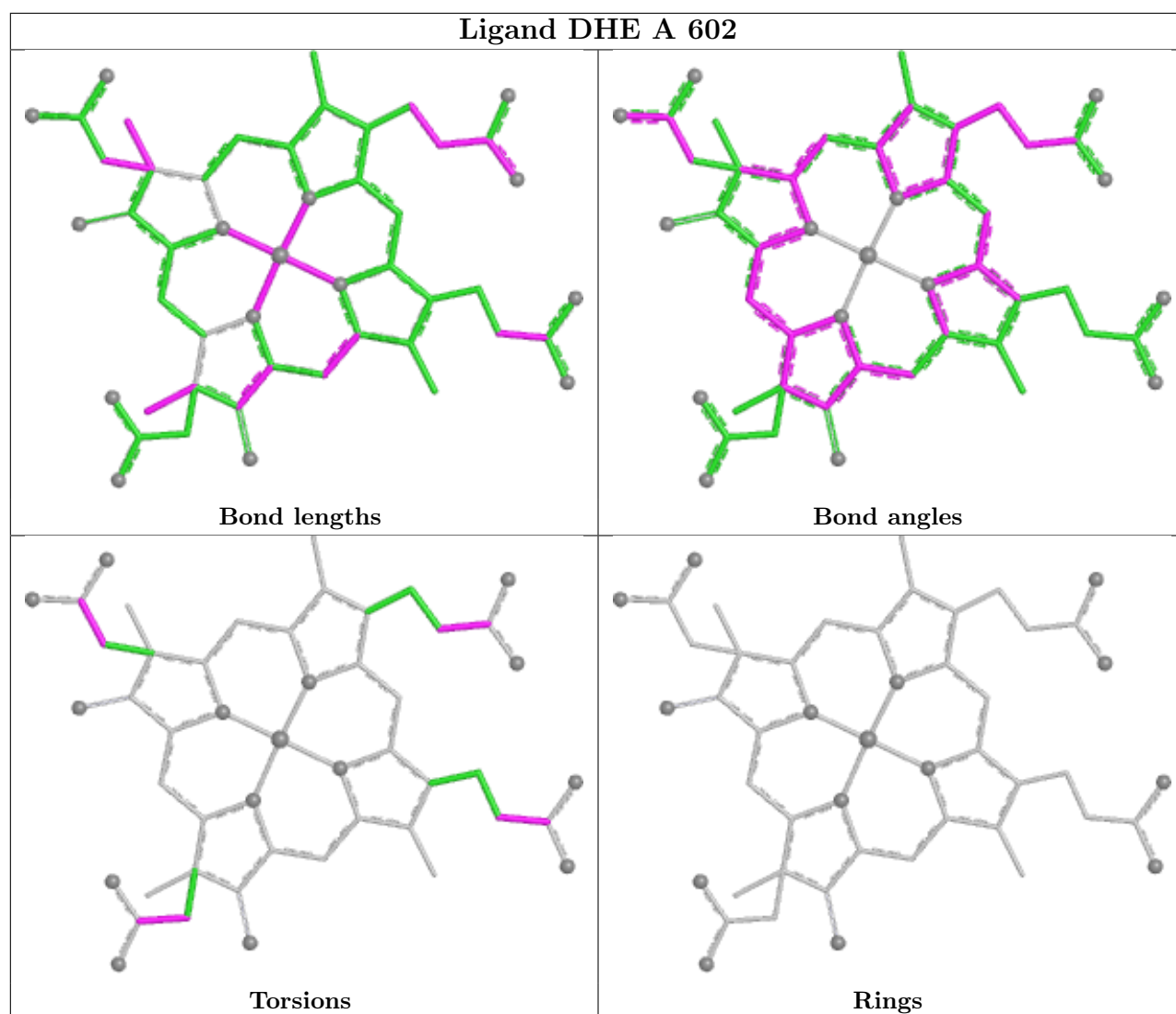
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEC	3	0
3	A	602	DHE	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](#)

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	514/543 (94%)	0.68	52 (10%)	12 10	38, 101, 173, 257	37 (7%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	ILE	5.4
1	A	114	PRO	5.1
1	A	74	GLN	5.0
1	A	72	GLY	4.8
1	A	36	PHE	4.4
1	A	109	ILE	4.4
1	A	65	PRO	4.1
1	A	445	ALA	4.0
1	A	75	TYR	4.0
1	A	116	PRO	3.9
1	A	524	PRO	3.9
1	A	43	TYR	3.8
1	A	57	GLY	3.7
1	A	64	THR	3.5
1	A	29	PRO	3.4
1	A	100	GLU	3.2
1	A	59	THR	3.1
1	A	28	ALA	3.0
1	A	423	SER	2.9
1	A	86	LEU	2.9
1	A	110	GLN	2.9
1	A	85	PRO	2.9
1	A	39	ALA	2.8
1	A	30	ASP	2.8
1	A	31	MET	2.7
1	A	232	PHE	2.7
1	A	81	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	432	SER	2.7
1	A	84	THR	2.6
1	A	63	LEU	2.6
1	A	120	GLY	2.6
1	A	52	GLY	2.6
1	A	393	GLY	2.6
1	A	87	GLY	2.5
1	A	413	VAL	2.5
1	A	451	VAL	2.4
1	A	408	TYR	2.4
1	A	96	GLU	2.3
1	A	440	THR	2.3
1	A	62	PRO	2.3
1	A	388	SER	2.3
1	A	83	GLY	2.3
1	A	454	PHE	2.2
1	A	105	MET	2.2
1	A	390	LEU	2.2
1	A	128	TRP	2.1
1	A	387	THR	2.1
1	A	108	TYR	2.1
1	A	53	VAL	2.0
1	A	102	ILE	2.0
1	A	279	GLU	2.0
1	A	23	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

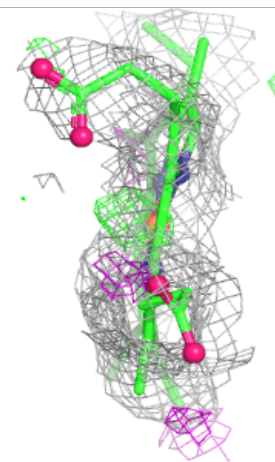
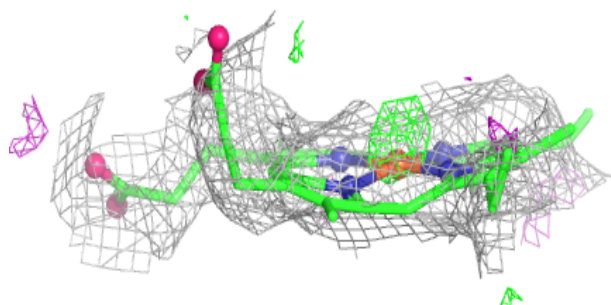
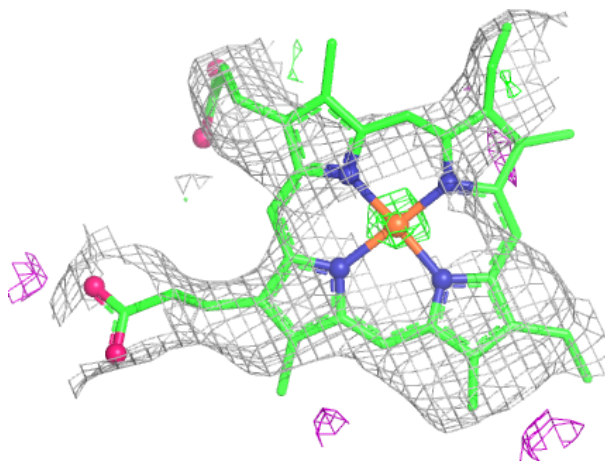
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEC	A	601	43/43	0.84	0.14	144,147,150,152	16
4	NO	A	603	2/2	0.88	0.16	60,60,60,63	0
3	DHE	A	602	49/49	0.93	0.11	66,74,79,81	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.

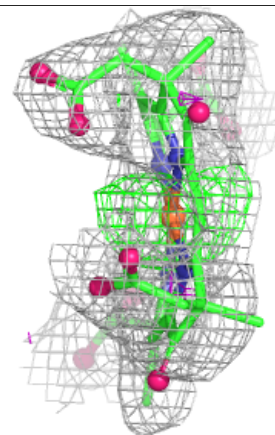
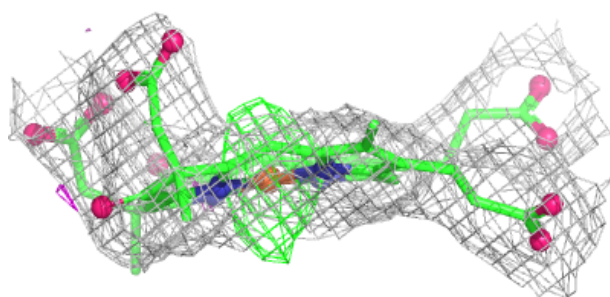
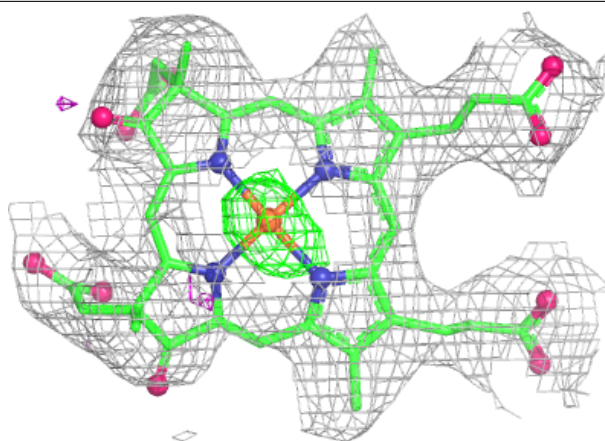
Electron density around HEC A 601:

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](#)

There are no such residues in this entry.