



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:33 PM UTC

PDB ID : 6XZ9 / pdb_00006xz9
Title : Structure of aldosterone synthase (CYP11B2) in complex with 5-chloro-3,3-dimethyl-2-[5-[1-(1-methylpyrazole-4-carbonyl)azetidin-3-yl]oxy-3-pyridyl]isoin-dolin-1-one
Authors : Kuglstatter, A.; Joseph, C.; Benz, J.
Deposited on : 2020-02-03
Resolution : 2.77 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

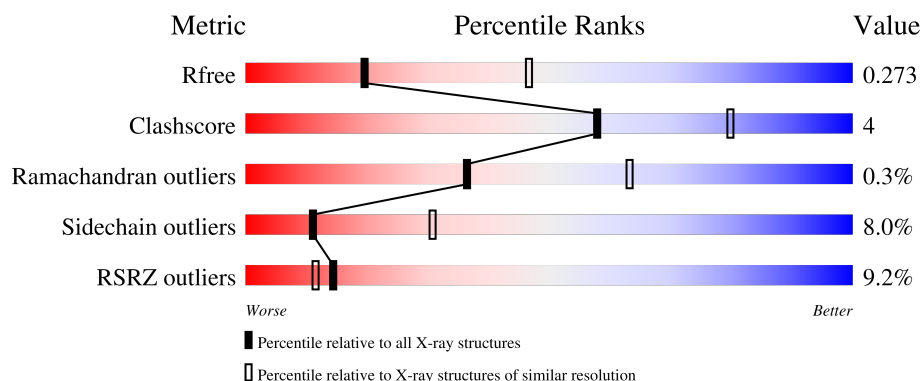
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	489	11% 80% 13% • 5%
1	B	489	6% 77% 17% • •
1	C	489	9% 76% 16% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11741 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome P450 11B2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3766	2433	665	648	20			
1	B	473	Total	C	N	O	S	0	0	0
			3832	2471	683	658	20			
1	C	466	Total	C	N	O	S	0	0	0
			3785	2445	670	650	20			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	initiating methionine	UNP P19099
A	25	ALA	-	expression tag	UNP P19099
A	26	THR	-	expression tag	UNP P19099
A	27	LYS	-	expression tag	UNP P19099
A	504	GLY	-	expression tag	UNP P19099
A	505	GLY	-	expression tag	UNP P19099
A	506	ARG	-	expression tag	UNP P19099
A	507	HIS	-	expression tag	UNP P19099
A	508	HIS	-	expression tag	UNP P19099
A	509	HIS	-	expression tag	UNP P19099
A	510	HIS	-	expression tag	UNP P19099
A	511	HIS	-	expression tag	UNP P19099
A	512	HIS	-	expression tag	UNP P19099
B	24	MET	-	initiating methionine	UNP P19099
B	25	ALA	-	expression tag	UNP P19099
B	26	THR	-	expression tag	UNP P19099
B	27	LYS	-	expression tag	UNP P19099
B	504	GLY	-	expression tag	UNP P19099
B	505	GLY	-	expression tag	UNP P19099
B	506	ARG	-	expression tag	UNP P19099
B	507	HIS	-	expression tag	UNP P19099
B	508	HIS	-	expression tag	UNP P19099
B	509	HIS	-	expression tag	UNP P19099

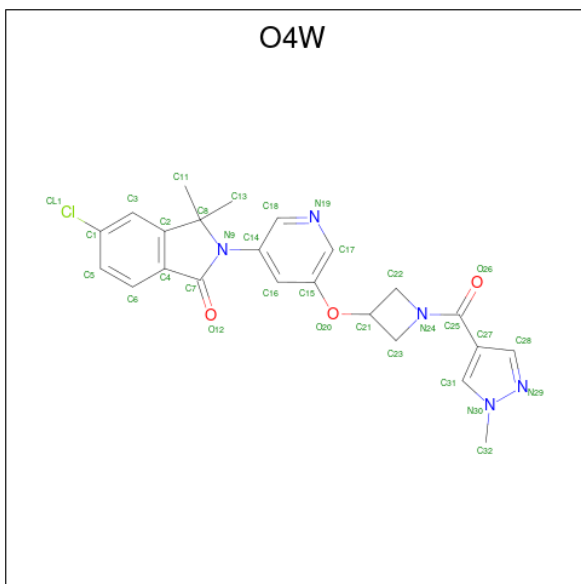
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Chain	Residue	Modelled	Actual	Comment	Reference
B	510	HIS	-	expression tag	UNP P19099
B	511	HIS	-	expression tag	UNP P19099
B	512	HIS	-	expression tag	UNP P19099
C	24	MET	-	initiating methionine	UNP P19099
C	25	ALA	-	expression tag	UNP P19099
C	26	THR	-	expression tag	UNP P19099
C	27	LYS	-	expression tag	UNP P19099
C	504	GLY	-	expression tag	UNP P19099
C	505	GLY	-	expression tag	UNP P19099
C	506	ARG	-	expression tag	UNP P19099
C	507	HIS	-	expression tag	UNP P19099
C	508	HIS	-	expression tag	UNP P19099
C	509	HIS	-	expression tag	UNP P19099
C	510	HIS	-	expression tag	UNP P19099
C	511	HIS	-	expression tag	UNP P19099
C	512	HIS	-	expression tag	UNP P19099

- [illegible]

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

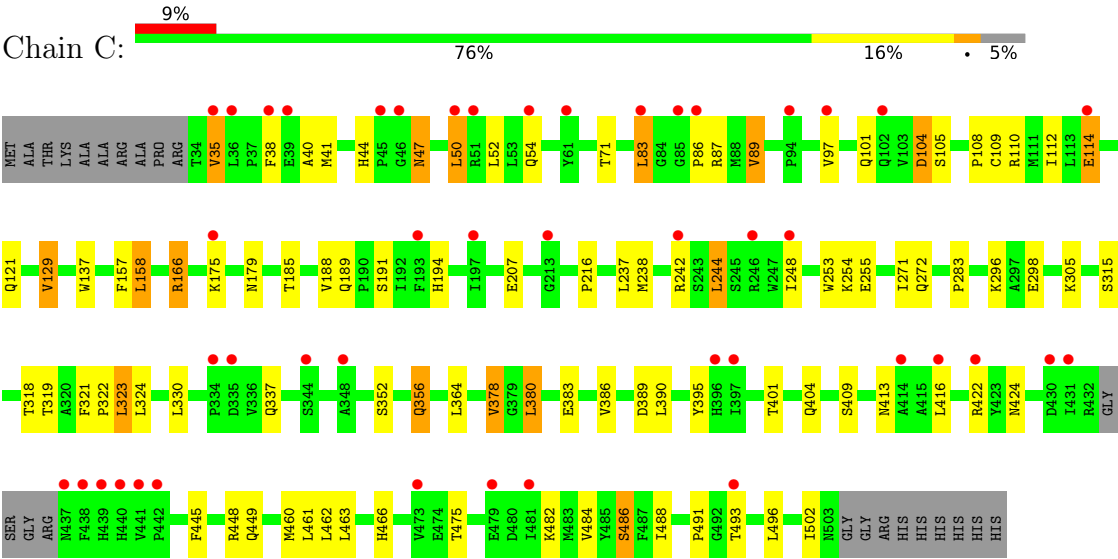
- Molecule 3 is 5-chloranyl-3,3-dimethyl-2-[5-[1-(1-methylpyrazol-4-yl)carbonylazetidino-3-yl]oxypyridin-3-yl]isoindol-1-one (CCD ID: O4W) (formula: C₂₃H₂₂ClN₅O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 32	C 23	Cl 1	N 5	O 3	0	0
3	B	1	Total 32	C 23	Cl 1	N 5	O 3	0	0
3	C	1	Total 32	C 23	Cl 1	N 5	O 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	42	Total O 42 42	0	0
4	B	48	Total O 48 48	0	0
4	C	43	Total O 43 43	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	107.68Å 121.60Å 298.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.58 – 2.77 48.58 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.58-2.77) 99.5 (48.58-2.77)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	0.30	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.234 , 0.273 (Not available) , 0.273	Depositor DCC
R_{free} test set	2539 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11741	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.81% 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, O4W

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	0/3866	1.36	13/5246 (0.2%)
1	B	0.79	0/3934	1.40	21/5336 (0.4%)
1	C	0.80	0/3885	1.38	25/5271 (0.5%)
All	All	0.80	0/11685	1.38	59/15853 (0.4%)

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	MET	N-CA-C	6.50	118.16	111.14
1	B	92	MET	N-CA-C	-6.48	99.80	108.74
1	C	237	LEU	CA-C-N	6.45	129.57	120.28
1	C	237	LEU	C-N-CA	6.45	129.57	120.28
1	B	437	ASN	CA-CB-CG	6.02	118.62	112.60
1	B	40	ALA	CA-C-N	5.87	128.54	120.39
1	B	40	ALA	C-N-CA	5.87	128.54	120.39
1	A	238	MET	N-CA-C	5.84	117.32	111.07
1	C	389	ASP	CA-CB-CG	5.82	118.42	112.60
1	B	254	LYS	CA-C-N	5.72	128.27	120.54
1	B	254	LYS	C-N-CA	5.72	128.27	120.54
1	C	35	VAL	N-CA-CB	5.72	116.96	110.72
1	A	254	LYS	CA-C-N	5.71	128.25	120.54
1	A	254	LYS	C-N-CA	5.71	128.25	120.54
1	C	254	LYS	CA-C-N	5.68	128.21	120.54
1	C	254	LYS	C-N-CA	5.68	128.21	120.54
1	A	157	PHE	CA-CB-CG	5.52	119.32	113.80
1	B	389	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	255	GLU	CA-C-N	5.39	127.77	120.44
1	B	255	GLU	C-N-CA	5.39	127.77	120.44
1	C	409	SER	CA-C-N	5.38	127.44	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	409	SER	C-N-CA	5.38	127.44	120.44
1	B	157	PHE	CA-CB-CG	5.26	119.06	113.80
1	A	269	ASN	CA-C-N	5.25	127.27	120.44
1	A	269	ASN	C-N-CA	5.25	127.27	120.44
1	A	305	LYS	CA-C-N	5.25	127.27	120.44
1	A	305	LYS	C-N-CA	5.25	127.27	120.44
1	A	237	LEU	CA-C-N	5.25	127.26	120.44
1	A	237	LEU	C-N-CA	5.25	127.26	120.44
1	A	389	ASP	CA-CB-CG	5.25	117.85	112.60
1	C	157	PHE	CA-CB-CG	5.24	119.04	113.80
1	C	97	VAL	CA-C-N	5.23	127.55	120.44
1	C	97	VAL	C-N-CA	5.23	127.55	120.44
1	B	288	GLY	CA-C-N	5.22	127.14	120.56
1	B	288	GLY	C-N-CA	5.22	127.14	120.56
1	B	114	GLU	CB-CG-CD	5.19	121.43	112.60
1	B	237	LEU	CA-C-N	5.18	127.48	120.44
1	B	237	LEU	C-N-CA	5.18	127.48	120.44
1	A	255	GLU	CA-C-N	5.17	127.48	120.44
1	A	255	GLU	C-N-CA	5.17	127.48	120.44
1	C	175	LYS	CA-C-N	5.16	127.07	120.56
1	C	175	LYS	C-N-CA	5.16	127.07	120.56
1	C	40	ALA	CA-C-N	5.15	127.55	120.39
1	C	40	ALA	C-N-CA	5.15	127.55	120.39
1	C	486	SER	CA-C-N	5.11	131.30	121.54
1	C	486	SER	C-N-CA	5.11	131.30	121.54
1	B	305	LYS	CA-C-N	5.11	127.08	120.44
1	B	305	LYS	C-N-CA	5.11	127.08	120.44
1	B	129	VAL	N-CA-CB	5.08	116.82	110.47
1	B	175	LYS	CA-C-N	5.06	126.94	120.56
1	B	175	LYS	C-N-CA	5.06	126.94	120.56
1	C	305	LYS	CA-C-N	5.06	127.02	120.44
1	C	305	LYS	C-N-CA	5.06	127.02	120.44
1	C	114	GLU	CB-CG-CD	5.06	121.19	112.60
1	C	47	ASN	CA-CB-CG	5.05	117.66	112.60
1	C	121	GLN	CA-C-N	5.05	127.00	120.44
1	C	121	GLN	C-N-CA	5.05	127.00	120.44
1	C	255	GLU	CA-C-N	5.01	127.25	120.44
1	C	255	GLU	C-N-CA	5.01	127.25	120.44

There are no chirality outliers.

There are no planarity outliers.

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	3766	0	3797	28	0
1	B	3832	0	3870	38	0
1	C	3785	0	3821	38	0
2	A	43	0	32	4	0
2	B	43	0	33	5	0
2	C	43	0	32	4	0
3	A	32	0	0	0	0
3	B	32	0	0	0	0
3	C	32	0	0	0	0
4	A	42	0	0	1	0
4	B	48	0	0	1	0
4	C	43	0	0	1	0
All	All	11741	0	11585	104	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 4.

All (104) 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:315:SER:HA	2:B:601:HEC:HMC1	1.64	0.79
1:C:386:VAL:HG21	1:C:390:LEU:HD22	1.67	0.77
1:A:315:SER:HA	2:A:601:HEC:HMC1	1.70	0.73
1:C:422:ARG:HD3	1:C:424:ASN:HB2	1.74	0.69
1:B:89:VAL:HG21	1:B:397:ILE:HD12	1.75	0.68
1:B:322:PRO:HD3	1:B:378:VAL:HG11	1.81	0.62
1:B:234:THR:O	1:B:238:MET:HB2	1.99	0.61
1:B:158:LEU:HD23	1:B:462:LEU:HD11	1.83	0.61
1:C:47:ASN:HB3	1:C:50:LEU:HB2	1.84	0.59
1:B:241:PRO:HD2	1:B:244:LEU:HD12	1.85	0.58
1:C:101:GLN:HG3	1:C:445:PHE:HD1	1.69	0.58
1:A:325:MET:HE3	1:A:491:PRO:HG3	1.86	0.57
1:C:108:PRO:HB2	1:C:448:ARG:HG3	1.87	0.56
2:C:601:HEC:HMC1	2:C:601:HEC:HBC3	1.86	0.56
1:C:283:PRO:HG2	4:C:714:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:MET:HE3	1:B:491:PRO:HG3	1.88	0.56
1:C:101:GLN:HG3	1:C:445:PHE:CD1	2.41	0.55
1:B:315:SER:CA	2:B:601:HEC:HMC1	2.37	0.55
4:B:723:HOH:O	1:C:179:ASN:HB3	2.07	0.54
1:C:158:LEU:HD23	1:C:462:LEU:HD11	1.90	0.54
1:C:378:VAL:HG23	2:C:601:HEC:HMB2	1.90	0.54
1:C:158:LEU:HD13	1:C:356:GLN:HA	1.90	0.53
1:C:321:PHE:CD2	1:C:491:PRO:HD2	2.44	0.53
1:B:328:PHE:CZ	1:B:332:ARG:HD2	2.45	0.52
1:B:408:TYR:O	1:B:412:ARG:HG2	2.09	0.52
1:C:315:SER:HB3	2:C:601:HEC:HBC3	1.91	0.52
1:B:101:GLN:O	1:B:104:ASP:HB2	2.10	0.52
1:B:321:PHE:CD2	1:B:491:PRO:HD2	2.46	0.51
1:A:321:PHE:CD2	1:A:491:PRO:HD2	2.46	0.51
1:C:244:LEU:HG	1:C:248:ILE:HD12	1.91	0.51
1:C:87:ARG:HB3	1:C:401:THR:HG23	1.93	0.51
1:A:158:LEU:HD13	1:A:356:GLN:HA	1.91	0.51
1:C:413:ASN:HB3	1:C:416:LEU:HD12	1.94	0.50
1:B:166:ARG:HH21	1:B:466:HIS:CE1	2.30	0.50
1:C:383:GLU:HG2	1:C:404:GLN:HG3	1.93	0.50
1:B:65:HIS:HB3	1:B:380:LEU:HD11	1.94	0.49
1:B:137:TRP:CZ2	1:B:448:ARG:HG2	2.47	0.49
1:A:38:PHE:HE1	1:A:89:VAL:HG22	1.77	0.49
1:A:413:ASN:HB3	1:A:416:LEU:HD12	1.95	0.49
1:A:158:LEU:HD23	1:A:462:LEU:HD11	1.95	0.49
1:B:70:GLN:HA	1:B:73:GLN:HE21	1.78	0.48
1:B:413:ASN:HB3	1:B:416:LEU:HD12	1.94	0.48
1:A:89:VAL:HG21	1:A:397:ILE:HD12	1.94	0.48
1:A:315:SER:CA	2:A:601:HEC:HMC1	2.42	0.48
1:A:330:LEU:HB3	1:A:337:GLN:HG3	1.96	0.48
1:A:296:LYS:HB3	1:A:298:GLU:HG3	1.96	0.48
1:B:315:SER:HA	2:B:601:HEC:CMC	2.40	0.47
1:A:110:ARG:HG3	4:A:707:HOH:O	2.15	0.47
1:C:330:LEU:HB3	1:C:337:GLN:HG3	1.96	0.47
1:C:41:MET:HA	1:C:395:TYR:CZ	2.49	0.47
1:C:101:GLN:O	1:C:104:ASP:HB2	2.13	0.47
1:C:110:ARG:HH22	2:C:601:HEC:HAD2	1.79	0.47
1:B:330:LEU:HB3	1:B:337:GLN:HG3	1.95	0.47
1:C:38:PHE:HE1	1:C:89:VAL:HG22	1.80	0.47
1:C:83:LEU:HD23	1:C:86:PRO:HB2	1.97	0.47
1:A:51:ARG:O	1:A:54:GLN:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:VAL:HG21	1:B:390:LEU:HD13	1.97	0.47
1:B:166:ARG:HH21	1:B:466:HIS:HE1	1.63	0.47
1:B:158:LEU:HD13	1:B:356:GLN:HA	1.97	0.46
1:A:315:SER:HA	2:A:601:HEC:CMC	2.43	0.46
1:B:296:LYS:HB3	1:B:298:GLU:HG3	1.96	0.46
1:B:44:HIS:CD2	1:B:71:THR:HG21	2.51	0.46
1:B:378:VAL:HG21	2:B:601:HEC:HBB3	1.97	0.46
1:C:296:LYS:HB3	1:C:298:GLU:HG3	1.97	0.46
1:B:311:LEU:HD21	1:B:451:LEU:HD13	1.98	0.46
1:B:38:PHE:HE1	1:B:89:VAL:CG2	2.28	0.45
1:B:93:LEU:HD23	1:B:416:LEU:HD11	1.97	0.45
1:C:44:HIS:CD2	1:C:71:THR:HG21	2.52	0.45
1:B:194:HIS:NE2	1:B:216:PRO:HB3	2.32	0.45
1:A:101:GLN:O	1:A:104:ASP:HB2	2.17	0.45
1:C:166:ARG:HH11	1:C:466:HIS:CE1	2.35	0.45
1:C:38:PHE:O	1:C:41:MET:HB2	2.17	0.45
1:A:44:HIS:CD2	1:A:71:THR:HG21	2.51	0.44
1:A:83:LEU:HD23	1:A:86:PRO:HB2	1.98	0.44
1:A:380:LEU:HD22	1:A:489:LEU:HB2	1.98	0.44
2:A:601:HEC:HBB3	2:A:601:HEC:HMB3	1.99	0.44
1:B:452:GLY:HA3	2:B:601:HEC:HBC2	2.00	0.44
1:C:166:ARG:HH11	1:C:466:HIS:HE1	1.65	0.44
1:B:280:PHE:HZ	1:C:475:THR:O	2.01	0.44
1:C:194:HIS:NE2	1:C:216:PRO:HB3	2.33	0.43
1:A:61:TYR:CE1	1:A:64:LEU:HD13	2.53	0.43
1:B:323:LEU:HG	1:B:460:MET:HG2	2.01	0.43
1:C:185:THR:HG22	1:C:496:LEU:HG	2.01	0.43
1:A:108:PRO:HB2	1:A:448:ARG:HG3	1.99	0.43
1:B:189:GLN:HG3	1:B:324:LEU:HD22	2.00	0.43
1:A:129:VAL:HG22	1:A:137:TRP:CD1	2.54	0.42
1:A:183:SER:HB3	1:A:500:ARG:HG3	2.01	0.42
1:B:61:TYR:CE1	1:B:64:LEU:HD13	2.53	0.42
1:C:129:VAL:HG22	1:C:137:TRP:CD1	2.55	0.42
1:C:41:MET:SD	1:C:89:VAL:HG13	2.60	0.42
1:A:194:HIS:NE2	1:A:216:PRO:HB3	2.35	0.41
1:A:323:LEU:HG	1:A:460:MET:HG2	2.02	0.41
1:B:386:VAL:HG21	1:B:390:LEU:HD22	2.02	0.41
1:C:323:LEU:HG	1:C:460:MET:HG2	2.02	0.41
1:A:141:ARG:HH21	1:A:149:LEU:HD22	1.86	0.41
1:C:318:THR:O	1:C:322:PRO:HD2	2.19	0.41
1:A:38:PHE:HE1	1:A:89:VAL:CG2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:LEU:HD12	1:B:106:LEU:HA	1.98	0.41
1:C:189:GLN:HG3	1:C:324:LEU:HD22	2.01	0.41
1:B:185:THR:HG22	1:B:496:LEU:HG	2.03	0.40
1:C:242:ARG:HD2	1:C:253:TRP:CZ2	2.56	0.40
1:A:443:PHE:CG	1:A:453:ARG:HG3	2.56	0.40
1:B:273:LYS:HE3	1:C:185:THR:O	2.22	0.40
1:A:318:THR:O	1:A:322:PRO:HD2	2.22	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	460/489 (94%)	446 (97%)	13 (3%)	1 (0%)	43	70
1	B	471/489 (96%)	456 (97%)	13 (3%)	2 (0%)	30	57
1	C	462/489 (94%)	445 (96%)	16 (4%)	1 (0%)	43	70
All	All	1393/1467 (95%)	1347 (97%)	42 (3%)	4 (0%)	36	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	LEU
1	B	380	LEU
1	C	380	LEU
1	B	93	LEU

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	409/426 (96%)	380 (93%)	29 (7%)	13	36
1	B	415/426 (97%)	382 (92%)	33 (8%)	11	31
1	C	411/426 (96%)	374 (91%)	37 (9%)	9	26
All	All	1235/1278 (97%)	1136 (92%)	99 (8%)	11	31

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LEU
1	A	52	LEU
1	A	54	GLN
1	A	83	LEU
1	A	104	ASP
1	A	112	ILE
1	A	114	GLU
1	A	129	VAL
1	A	158	LEU
1	A	166	ARG
1	A	188	VAL
1	A	191	SER
1	A	207	GLU
1	A	246	ARG
1	A	271	ILE
1	A	323	LEU
1	A	352	SER
1	A	356	GLN
1	A	378	VAL
1	A	380	LEU
1	A	388	SER
1	A	421	GLU
1	A	426	GLN
1	A	449	GLN
1	A	463	LEU
1	A	482	LYS
1	A	484	VAL
1	A	488	ILE
1	A	493	THR
1	B	50	LEU

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Mol	Chain	Res	Type
1	B	51	ARG
1	B	82	ASN
1	B	101	GLN
1	B	105	SER
1	B	109	CYS
1	B	112	ILE
1	B	113	LEU
1	B	114	GLU
1	B	120	ARG
1	B	129	VAL
1	B	152	LYS
1	B	158	LEU
1	B	166	ARG
1	B	170	GLN
1	B	188	VAL
1	B	191	SER
1	B	207	GLU
1	B	221	LEU
1	B	317	ASP
1	B	323	LEU
1	B	352	SER
1	B	386	VAL
1	B	422	ARG
1	B	426	GLN
1	B	434	SER
1	B	449	GLN
1	B	451	LEU
1	B	461	LEU
1	B	463	LEU
1	B	478	GLN
1	B	479	GLU
1	B	493	THR
1	C	35	VAL
1	C	50	LEU
1	C	52	LEU
1	C	54	GLN
1	C	83	LEU
1	C	89	VAL
1	C	104	ASP
1	C	105	SER
1	C	109	CYS
1	C	112	ILE

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Mol	Chain	Res	Type
1	C	114	GLU
1	C	129	VAL
1	C	158	LEU
1	C	166	ARG
1	C	188	VAL
1	C	191	SER
1	C	207	GLU
1	C	238	MET
1	C	244	LEU
1	C	271	ILE
1	C	272	GLN
1	C	319	THR
1	C	323	LEU
1	C	352	SER
1	C	356	GLN
1	C	364	LEU
1	C	378	VAL
1	C	380	LEU
1	C	449	GLN
1	C	461	LEU
1	C	463	LEU
1	C	482	LYS
1	C	484	VAL
1	C	486	SER
1	C	488	ILE
1	C	493	THR
1	C	502	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	107	HIS
1	A	125	HIS
1	A	356	GLN
1	A	394	ASN
1	A	437	ASN
1	A	440	HIS
1	B	73	GLN
1	B	107	HIS
1	B	125	HIS
1	B	155	GLN

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Mol	Chain	Res	Type
1	B	170	GLN
1	B	236	GLN
1	B	356	GLN
1	B	394	ASN
1	B	440	HIS
1	B	478	GLN
1	C	47	ASN
1	C	73	GLN
1	C	107	HIS
1	C	155	GLN
1	C	214	HIS
1	C	356	GLN
1	C	440	HIS
1	C	466	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	O4W	A	602	2	36,36,36	1.12	2 (5%)	42,55,55	3.62	17 (40%)
3	O4W	B	602	2	36,36,36	1.14	2 (5%)	42,55,55	3.56	16 (38%)
3	O4W	C	602	2	36,36,36	1.25	3 (8%)	42,55,55	3.90	15 (35%)
2	HEC	A	601	3,1	46,50,50	1.63	5 (10%)	58,82,82	1.53	10 (17%)
2	HEC	B	601	3,1	46,50,50	1.85	11 (23%)	58,82,82	1.50	9 (15%)
2	HEC	C	601	3,1	46,50,50	1.73	11 (23%)	58,82,82	1.40	6 (10%)

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
3	O4W	A	602	2	-	6/16/44/44	0/5/5/5
3	O4W	B	602	2	-	3/16/44/44	0/5/5/5
3	O4W	C	602	2	-	4/16/44/44	0/5/5/5
2	HEC	A	601	3,1	-	4/14/54/54	-
2	HEC	B	601	3,1	-	6/14/54/54	-
2	HEC	C	601	3,1	-	2/14/54/54	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	O4W	N30-N29	5.04	1.41	1.35
2	A	601	HEC	CBC-CAC	-4.90	1.31	1.49
2	B	601	HEC	CAB-C3B	4.61	1.50	1.35
2	A	601	HEC	CAB-C3B	4.42	1.49	1.35
2	B	601	HEC	CBB-CAB	-4.38	1.33	1.49
2	C	601	HEC	CBB-CAB	-4.36	1.33	1.49
2	C	601	HEC	CBC-CAC	-4.15	1.34	1.49
3	A	602	O4W	N30-N29	4.14	1.40	1.35
2	B	601	HEC	CBC-CAC	-4.07	1.34	1.49
2	C	601	HEC	CAB-C3B	3.96	1.47	1.35
3	B	602	O4W	N30-N29	3.94	1.40	1.35
2	B	601	HEC	C3D-C2D	-3.86	1.28	1.38
2	A	601	HEC	CAC-C3C	3.74	1.47	1.35
2	A	601	HEC	CBB-CAB	-3.72	1.35	1.49
2	B	601	HEC	CAC-C3C	3.57	1.46	1.35
2	C	601	HEC	C3B-C4B	3.52	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	O4W	C7-N9	-3.14	1.34	1.38
2	C	601	HEC	CAC-C3C	3.01	1.44	1.35
2	B	601	HEC	C4B-NB	-3.01	1.34	1.39
2	C	601	HEC	C1D-C2D	2.82	1.49	1.43
3	C	602	O4W	C7-N9	-2.72	1.35	1.38
3	A	602	O4W	C7-N9	-2.61	1.35	1.38
2	B	601	HEC	C4D-ND	-2.49	1.34	1.39
2	C	601	HEC	C1A-C2A	-2.48	1.40	1.45
2	B	601	HEC	O2A-CGA	2.42	1.38	1.30
2	C	601	HEC	CBD-CGD	2.41	1.56	1.50
2	B	601	HEC	C3B-C4B	2.30	1.50	1.46
2	B	601	HEC	C4D-C3D	2.25	1.49	1.44
2	C	601	HEC	C1D-ND	-2.24	1.35	1.39
2	C	601	HEC	C4D-C3D	2.21	1.49	1.44
2	B	601	HEC	CHD-C1D	2.11	1.44	1.39
2	A	601	HEC	C1D-ND	-2.09	1.35	1.39
3	C	602	O4W	C14-N9	-2.08	1.39	1.43
2	C	601	HEC	CAA-C2A	-2.08	1.46	1.51

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	O4W	C23-N24-C22	-13.75	85.06	94.69
3	C	602	O4W	C23-N24-C22	-13.44	85.28	94.69
3	B	602	O4W	C23-N24-C22	-13.17	85.47	94.69
3	C	602	O4W	C28-N29-N30	9.85	109.82	104.41
3	C	602	O4W	C32-N30-N29	8.99	127.24	120.03
3	B	602	O4W	C32-N30-N29	8.62	126.94	120.03
3	A	602	O4W	C4-C7-N9	8.32	111.18	106.10
3	C	602	O4W	C31-N30-N29	-7.98	107.55	112.08
3	A	602	O4W	C32-N30-N29	7.86	126.33	120.03
3	C	602	O4W	C4-C7-N9	7.69	110.80	106.10
3	B	602	O4W	C4-C7-N9	7.61	110.75	106.10
3	A	602	O4W	C28-N29-N30	6.90	108.20	104.41
3	B	602	O4W	C28-N29-N30	6.87	108.18	104.41
3	B	602	O4W	C31-N30-N29	-6.05	108.64	112.08
3	C	602	O4W	C27-C28-N29	-5.83	107.46	112.09
3	A	602	O4W	C31-N30-N29	-5.68	108.86	112.08
3	C	602	O4W	C3-C2-C8	5.25	134.08	126.46
3	A	602	O4W	C3-C2-C8	5.12	133.90	126.46
2	A	601	HEC	O2D-CGD-O1D	-4.72	111.20	123.33
3	B	602	O4W	C3-C2-C8	4.66	133.23	126.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	HEC	CBC-CAC-C3C	-4.58	118.28	127.43
2	C	601	HEC	O2D-CGD-O1D	-4.29	112.30	123.33
3	A	602	O4W	C8-N9-C14	4.27	127.65	123.21
3	B	602	O4W	C27-C28-N29	-4.08	108.85	112.09
3	B	602	O4W	C8-N9-C14	3.78	127.14	123.21
3	A	602	O4W	C27-C28-N29	-3.74	109.12	112.09
3	C	602	O4W	C31-C27-C28	3.65	107.44	104.22
3	B	602	O4W	C32-N30-C31	-3.51	124.42	127.94
2	A	601	HEC	O2D-CGD-CBD	3.42	124.79	114.00
3	A	602	O4W	C18-C14-N9	3.38	123.25	119.60
2	B	601	HEC	CAA-C2A-C3A	-3.38	121.54	127.87
2	B	601	HEC	O2D-CGD-O1D	-3.32	114.79	123.33
3	A	602	O4W	C18-N19-C17	3.32	122.02	117.51
3	B	602	O4W	C18-N19-C17	3.28	121.97	117.51
3	A	602	O4W	O12-C7-C4	-3.23	122.41	128.66
2	B	601	HEC	O2D-CGD-CBD	3.21	124.15	114.00
3	A	602	O4W	C32-N30-C31	-3.19	124.73	127.94
3	C	602	O4W	C21-C23-N24	-3.16	84.83	87.96
3	C	602	O4W	C21-C22-N24	-3.15	84.83	87.96
2	C	601	HEC	CBA-CAA-C2A	-3.15	103.83	112.53
3	C	602	O4W	O12-C7-C4	-2.96	122.92	128.66
2	C	601	HEC	O2D-CGD-CBD	2.91	123.18	114.00
2	A	601	HEC	O2A-CGA-CBA	2.76	122.73	114.00
3	C	602	O4W	C32-N30-C31	-2.73	125.20	127.94
2	C	601	HEC	CBC-CAC-C3C	-2.72	122.01	127.43
2	A	601	HEC	CMD-C2D-C3D	2.68	131.31	125.62
3	B	602	O4W	C21-C22-N24	-2.64	85.34	87.96
2	A	601	HEC	CHD-C1D-C2D	-2.63	119.79	127.43
2	A	601	HEC	CAA-C2A-C3A	-2.60	122.99	127.87
2	B	601	HEC	CAA-C2A-C1A	2.53	129.99	124.85
3	C	602	O4W	C18-C14-N9	2.49	122.30	119.60
3	C	602	O4W	C18-N19-C17	2.49	120.89	117.51
2	A	601	HEC	CHC-C4B-NB	2.47	127.14	124.45
2	A	601	HEC	CBC-CAC-C3C	-2.44	122.55	127.43
3	A	602	O4W	O26-C25-N24	-2.43	118.84	122.67
3	B	602	O4W	C13-C8-C2	-2.42	108.41	112.15
2	B	601	HEC	CHD-C1D-C2D	-2.41	120.42	127.43
2	A	601	HEC	O2A-CGA-O1A	-2.36	117.25	123.33
2	B	601	HEC	CAD-CBD-CGD	-2.35	107.43	113.67
3	C	602	O4W	O26-C25-N24	-2.34	118.97	122.67
3	A	602	O4W	C21-C22-N24	-2.31	85.67	87.96
3	B	602	O4W	O12-C7-N9	-2.31	123.83	125.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	O4W	C21-C23-N24	-2.24	85.74	87.96
2	C	601	HEC	C4A-NA-C1A	-2.21	102.22	105.82
2	B	601	HEC	C4D-ND-C1D	-2.14	102.33	105.82
3	B	602	O4W	C31-C27-C28	2.14	106.11	104.22
3	A	602	O4W	C13-C8-C2	-2.13	108.86	112.15
2	C	601	HEC	C3D-C4D-ND	2.12	112.50	110.15
3	A	602	O4W	C13-C8-C11	-2.09	106.02	110.20
3	B	602	O4W	C18-C14-N9	2.08	121.85	119.60
2	B	601	HEC	O2A-CGA-CBA	2.06	120.50	114.00
2	A	601	HEC	CHD-C1D-ND	2.05	127.58	123.86
3	B	602	O4W	C21-C23-N24	-2.01	85.96	87.96

There are no chirality outliers.

All (25) torsion outliers are listed below:

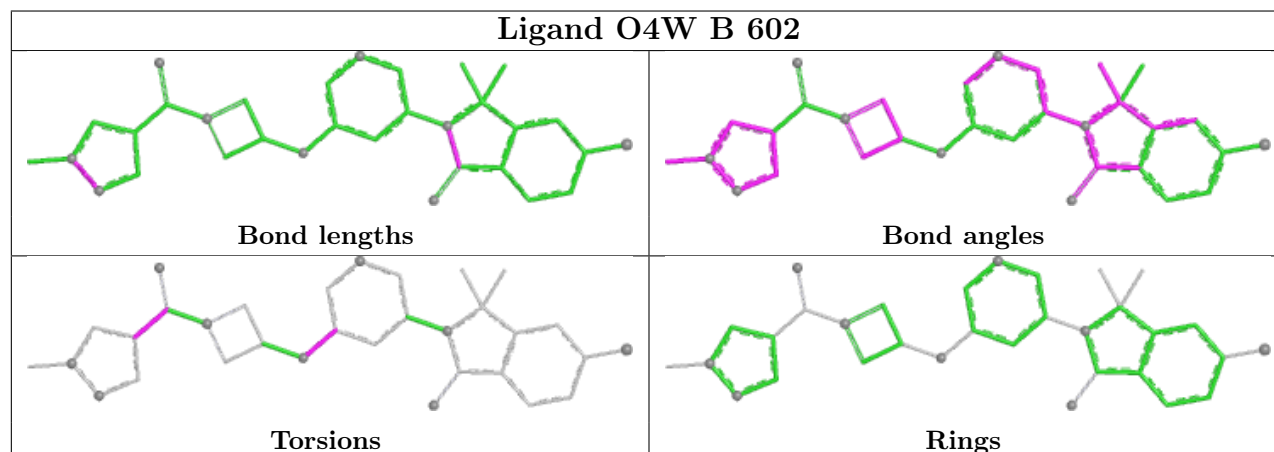
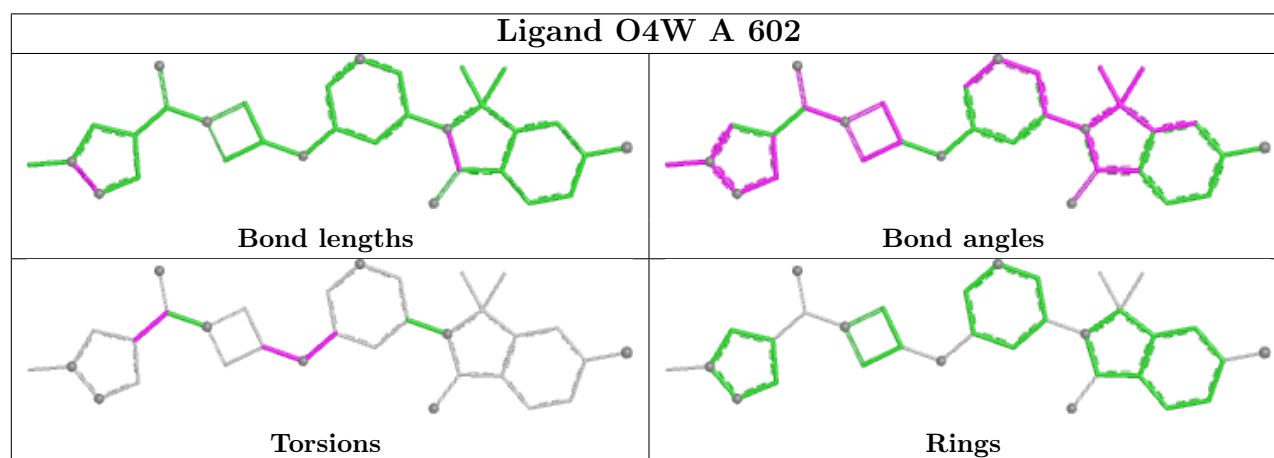
Mol	Chain	Res	Type	Atoms
2	A	601	HEC	C2B-C3B-CAB-CBB
2	A	601	HEC	C4B-C3B-CAB-CBB
2	A	601	HEC	C2C-C3C-CAC-CBC
2	A	601	HEC	C4C-C3C-CAC-CBC
2	B	601	HEC	C2B-C3B-CAB-CBB
2	B	601	HEC	C4B-C3B-CAB-CBB
2	B	601	HEC	C2C-C3C-CAC-CBC
2	B	601	HEC	C4C-C3C-CAC-CBC
2	C	601	HEC	C2C-C3C-CAC-CBC
2	C	601	HEC	C4C-C3C-CAC-CBC
3	A	602	O4W	N24-C25-C27-C31
3	C	602	O4W	C17-C15-O20-C21
3	B	602	O4W	C17-C15-O20-C21
3	B	602	O4W	C16-C15-O20-C21
3	A	602	O4W	C17-C15-O20-C21
3	A	602	O4W	C16-C15-O20-C21
3	C	602	O4W	C16-C15-O20-C21
2	B	601	HEC	CAD-CBD-CGD-O2D
2	B	601	HEC	CAD-CBD-CGD-O1D
3	A	602	O4W	O26-C25-C27-C31
3	B	602	O4W	N24-C25-C27-C31
3	C	602	O4W	N24-C25-C27-C31
3	A	602	O4W	C22-C21-O20-C15
3	A	602	O4W	C23-C21-O20-C15
3	C	602	O4W	C23-C21-O20-C15

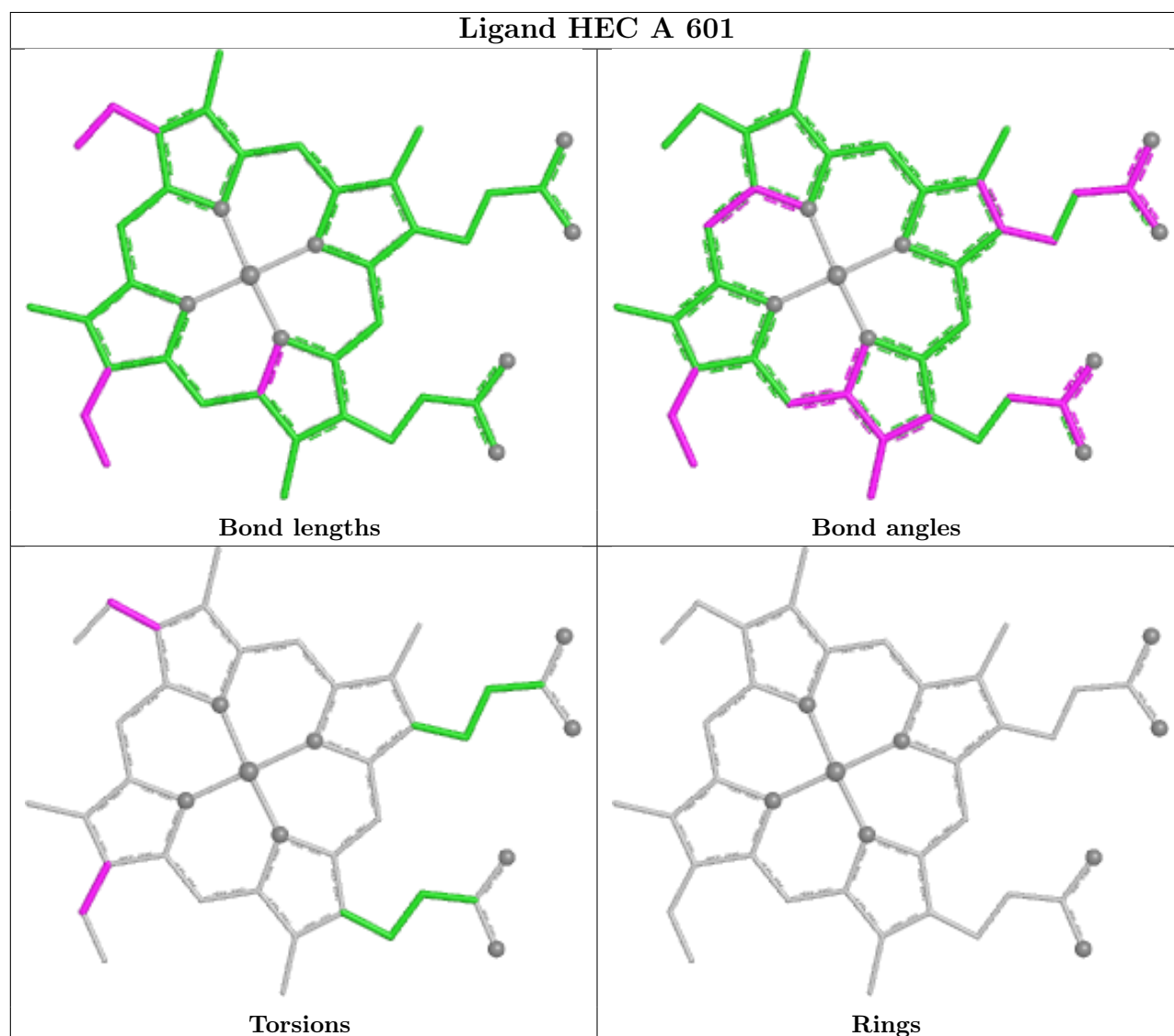
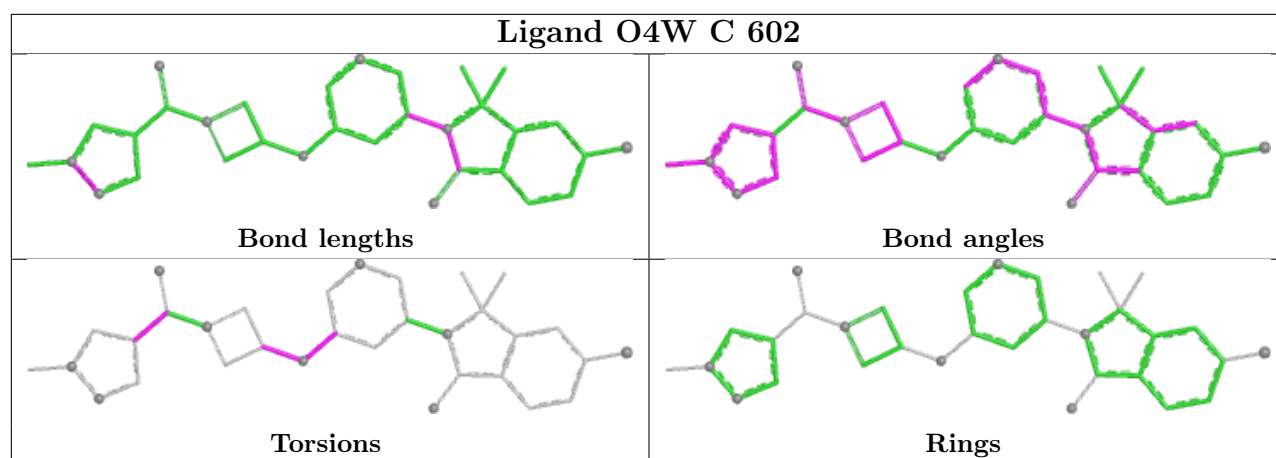
There are no ring outliers.

3 monomers are involved in 13 short contacts:

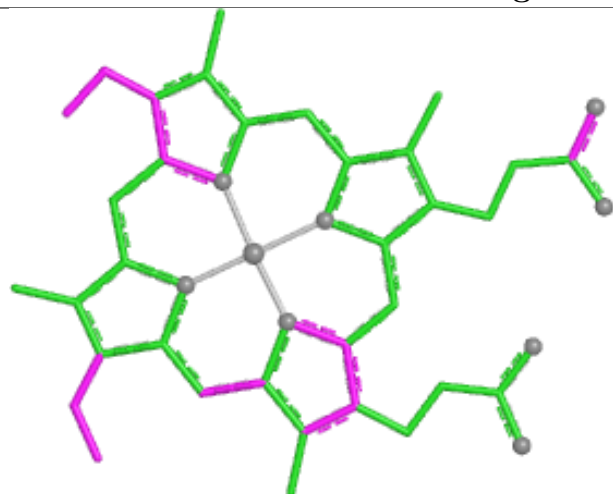
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEC	4	0
2	B	601	HEC	5	0
2	C	601	HEC	4	0

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

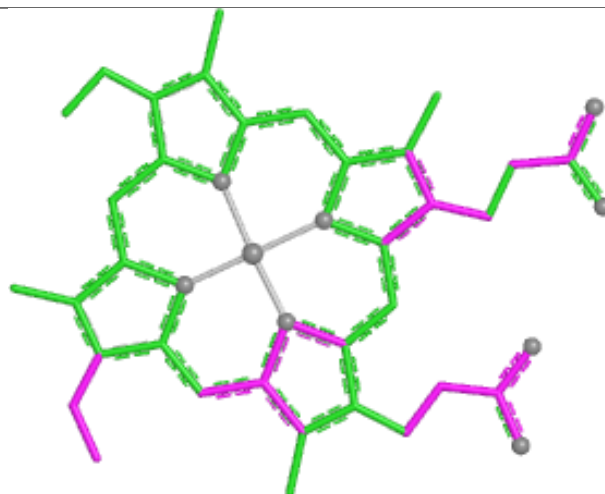




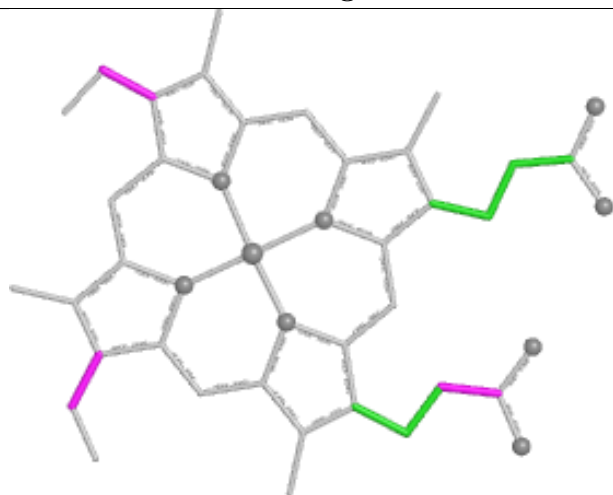
Ligand HEC B 601



Bond lengths



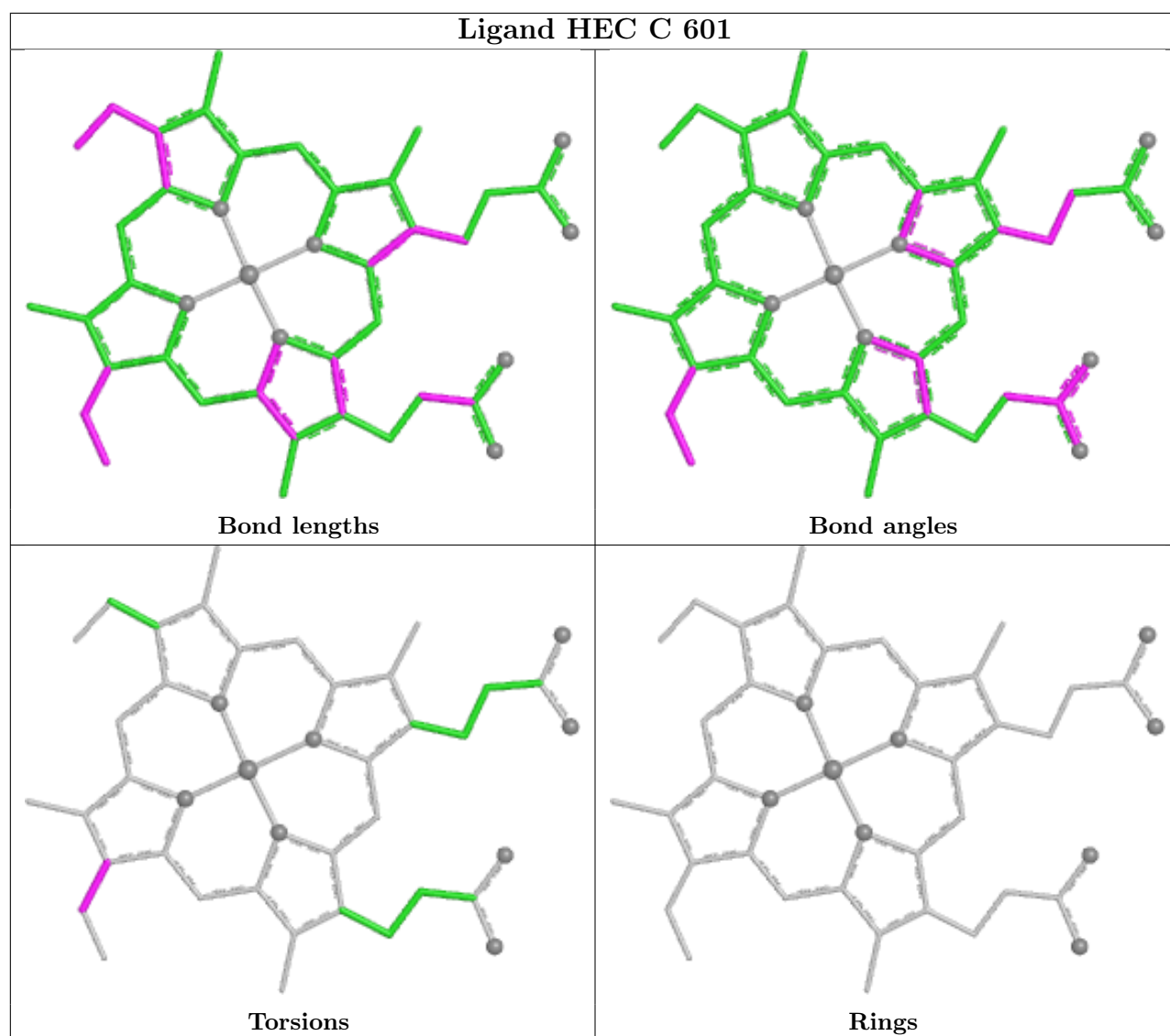
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	464/489 (94%)	1.07	53 (11%) 10 8	33, 52, 79, 101	0
1	B	473/489 (96%)	0.89	31 (6%) 24 19	29, 47, 70, 98	0
1	C	466/489 (95%)	1.00	45 (9%) 13 10	32, 49, 73, 106	0
All	All	1403/1467 (95%)	0.99	129 (9%) 14 11	29, 50, 74, 106	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	431	ILE	4.8
1	A	112	ILE	4.0
1	B	504	GLY	4.0
1	C	35	VAL	3.7
1	A	56	TRP	3.7
1	A	358	ALA	3.7
1	C	396	HIS	3.5
1	A	34	THR	3.5
1	C	416	LEU	3.4
1	C	438	PHE	3.4
1	B	431	ILE	3.4
1	B	358	ALA	3.3
1	B	83	LEU	3.2
1	C	94	PRO	3.2
1	C	36	LEU	3.1
1	B	421	GLU	3.1
1	A	477	THR	3.0
1	B	46	GLY	2.9
1	C	442	PRO	2.9
1	A	50	LEU	2.9
1	C	440	HIS	2.9
1	A	479	GLU	2.8
1	B	430	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	97	VAL	2.8
1	B	32	PRO	2.8
1	C	51	ARG	2.8
1	B	177	LEU	2.8
1	C	175	LYS	2.8
1	B	49	TRP	2.8
1	A	307	ASN	2.8
1	A	430	ASP	2.8
1	C	397	ILE	2.7
1	A	52	LEU	2.7
1	A	114	GLU	2.7
1	C	414	ALA	2.7
1	C	86	PRO	2.7
1	B	82	ASN	2.7
1	C	61	TYR	2.7
1	A	83	LEU	2.6
1	B	502	ILE	2.6
1	B	314	GLY	2.6
1	B	442	PRO	2.6
1	A	437	ASN	2.6
1	C	437	ASN	2.6
1	A	63	HIS	2.6
1	A	175	LYS	2.6
1	C	193	PHE	2.5
1	C	344	SER	2.5
1	A	419	ARG	2.5
1	C	39	GLU	2.5
1	A	441	VAL	2.5
1	C	430	ASP	2.5
1	A	231	PHE	2.5
1	A	324	LEU	2.5
1	A	97	VAL	2.5
1	B	170	GLN	2.5
1	C	50	LEU	2.4
1	A	291	ALA	2.4
1	A	503	ASN	2.4
1	C	439	HIS	2.4
1	B	152	LYS	2.4
1	C	46	GLY	2.4
1	A	129	VAL	2.4
1	C	83	LEU	2.4
1	A	335	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	51	ARG	2.3
1	A	396	HIS	2.3
1	C	493	THR	2.3
1	C	114	GLU	2.3
1	A	49	TRP	2.3
1	C	422	ARG	2.3
1	C	441	VAL	2.3
1	C	38	PHE	2.3
1	C	481	ILE	2.3
1	A	47	ASN	2.3
1	B	467	VAL	2.3
1	A	345	LEU	2.3
1	A	416	LEU	2.3
1	B	215	SER	2.3
1	A	446	GLY	2.3
1	B	158	LEU	2.3
1	A	248	ILE	2.2
1	A	493	THR	2.2
1	C	102	GLN	2.2
1	C	335	ASP	2.2
1	A	115	PRO	2.2
1	B	355	PRO	2.2
1	A	303	ALA	2.2
1	B	40	ALA	2.2
1	B	432	ARG	2.2
1	A	124	GLY	2.2
1	A	244	LEU	2.2
1	C	85	GLY	2.2
1	C	213	GLY	2.2
1	A	494	SER	2.2
1	C	473	VAL	2.2
1	B	34	THR	2.2
1	C	242	ARG	2.2
1	B	33	ARG	2.1
1	A	111	MET	2.1
1	A	364	LEU	2.1
1	B	209	LEU	2.1
1	C	248	ILE	2.1
1	C	246	ARG	2.1
1	A	121	GLN	2.1
1	A	85	GLY	2.1
1	A	122	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	214	HIS	2.1
1	C	479	GLU	2.1
1	A	46	GLY	2.1
1	A	438	PHE	2.1
1	B	443	PHE	2.1
1	B	218	SER	2.1
1	B	359	THR	2.1
1	C	334	PRO	2.1
1	C	197	ILE	2.1
1	B	188	VAL	2.1
1	A	239	PHE	2.1
1	A	412	ARG	2.0
1	A	99	LYS	2.0
1	A	126	LYS	2.0
1	A	297	ALA	2.0
1	C	348	ALA	2.0
1	A	191	SER	2.0
1	A	151	PRO	2.0
1	C	45	PRO	2.0
1	A	178	GLN	2.0
1	B	301	LEU	2.0
1	C	54	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	O4W	A	602	32/32	0.80	0.18	56,61,73,88	0

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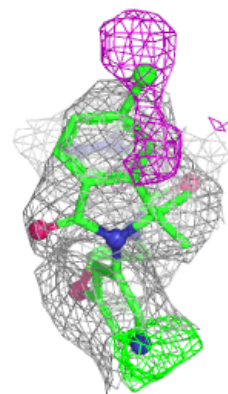
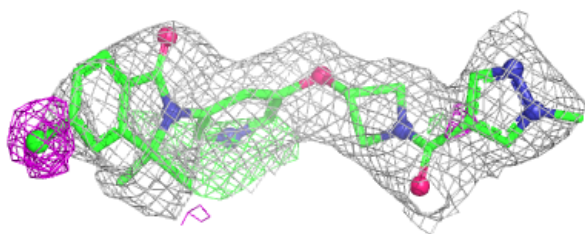
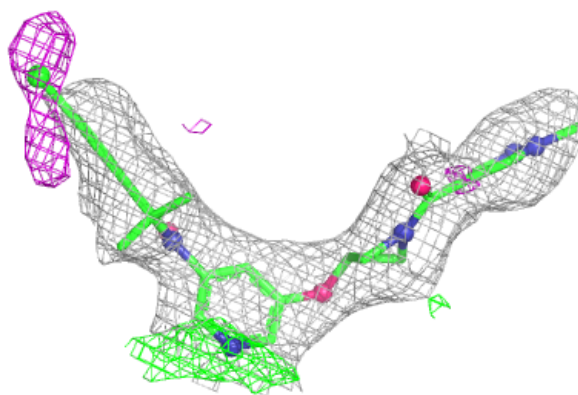
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	O4W	C	602	32/32	0.89	0.12	35,42,52,68	0
3	O4W	B	602	32/32	0.90	0.13	33,47,55,70	0
2	HEC	A	601	43/43	0.94	0.13	44,45,49,53	0
2	HEC	C	601	43/43	0.95	0.11	39,40,44,46	0
2	HEC	B	601	43/43	0.96	0.10	32,34,39,39	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.

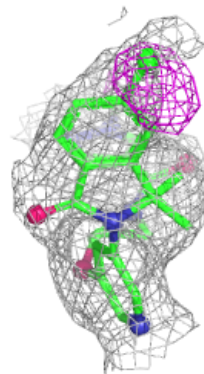
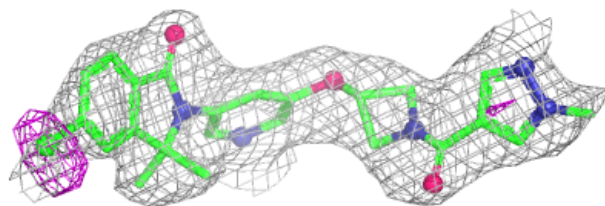
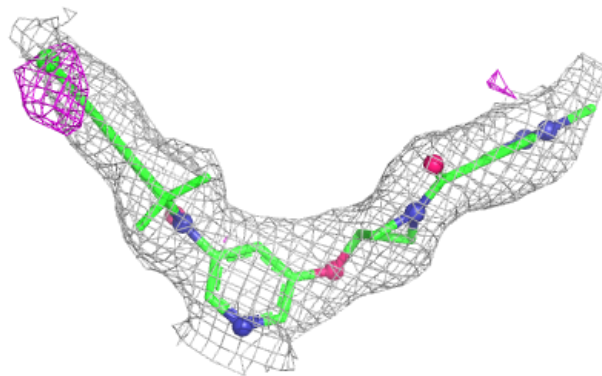
Electron density around O4W A 602:

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

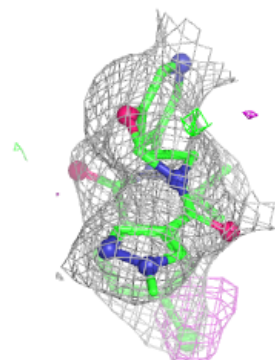
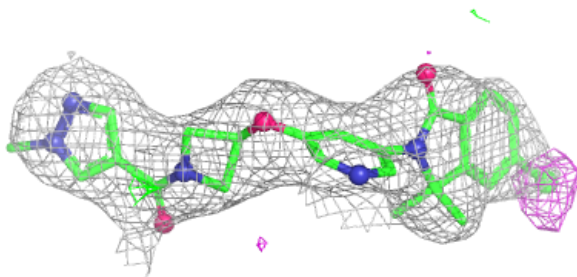
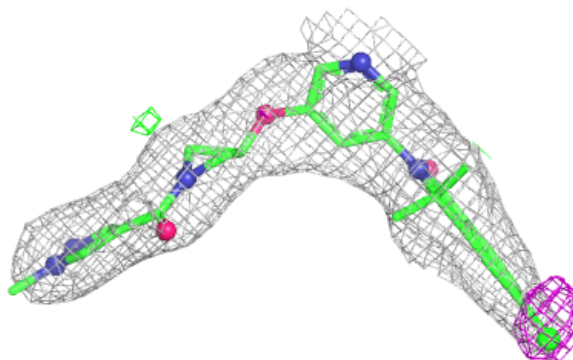


Electron density around O4W C 602:

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

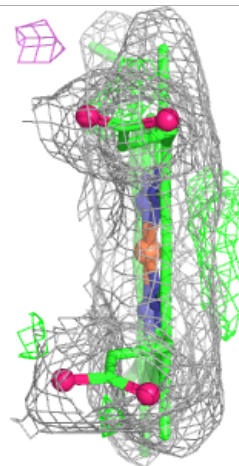
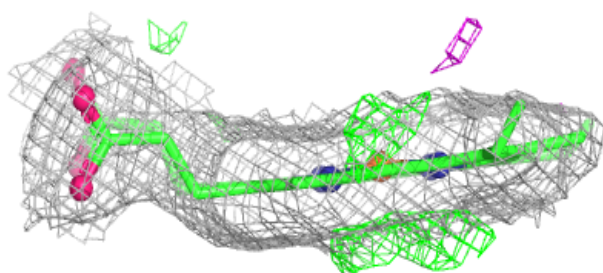
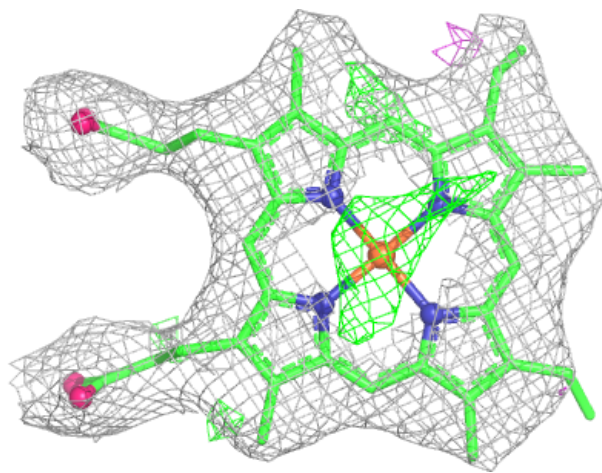
**Electron density around O4W B 602:**

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



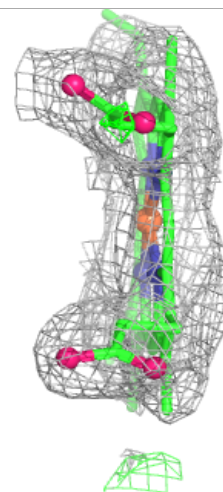
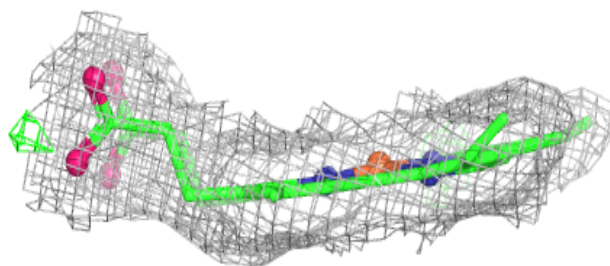
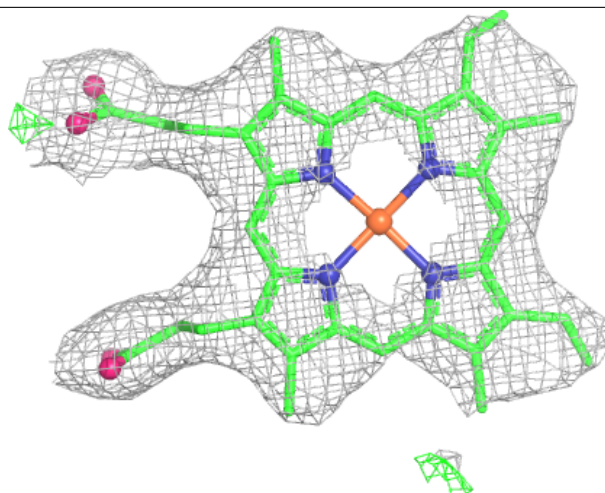
Electron density around HEC A 601:

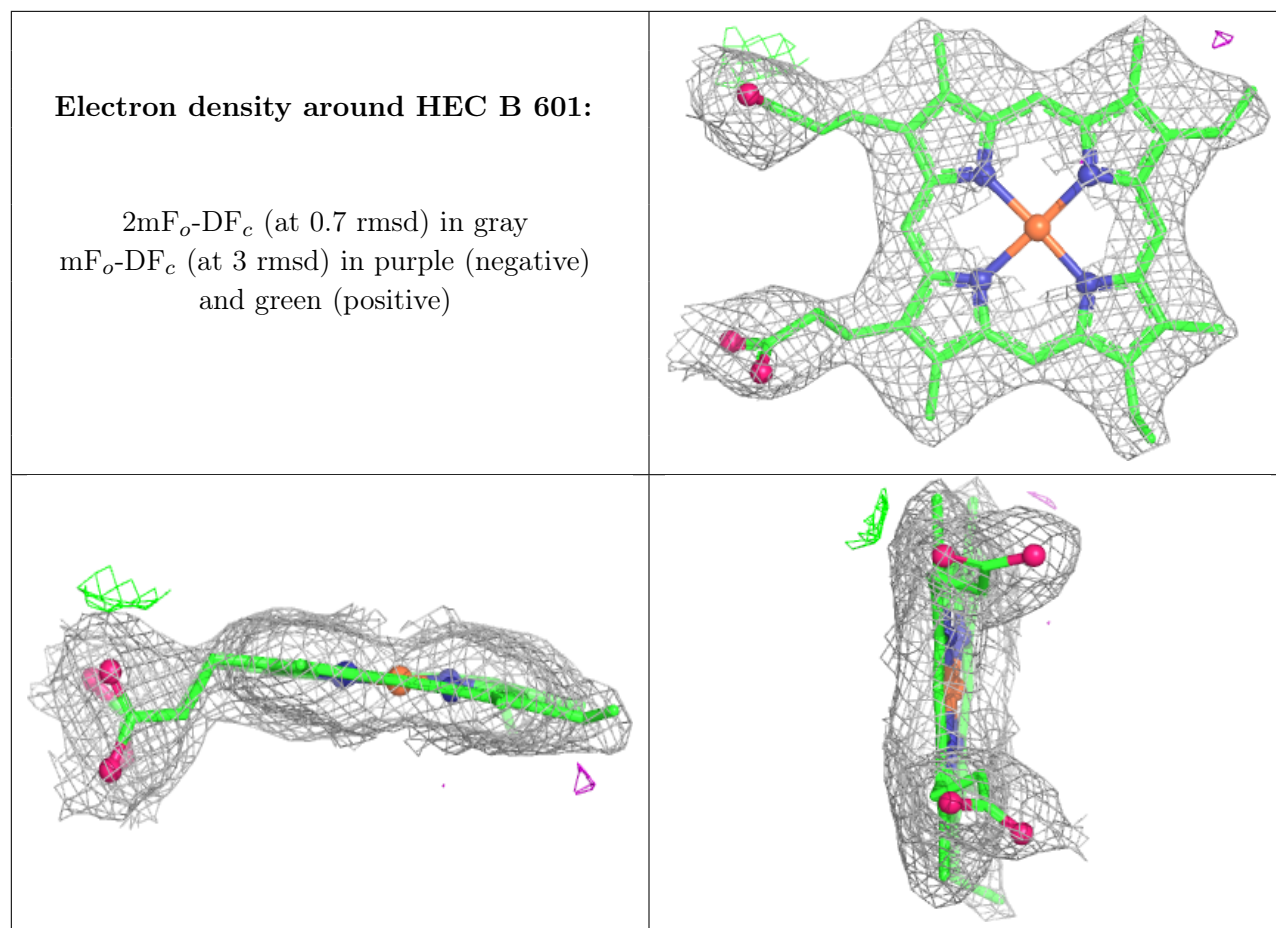
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC C 601:

$2mF_o-DF_c$ (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.