



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2024 – 06:25 pm BST

PDB ID : 6XZ8
Title : Structure of aldosterone synthase (CYP11B2) in complex with N-[(1R)-1-[5-(6-chloro-1,1-dimethyl-3-oxo-isoindolin-2-yl)-3-pyridyl]ethyl]methanesulfonamide
Authors : Kuglstatter, A.; Joseph, C.; Benz, J.
Deposited on : 2020-02-03
Resolution : 3.00 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
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) : 2.36.2

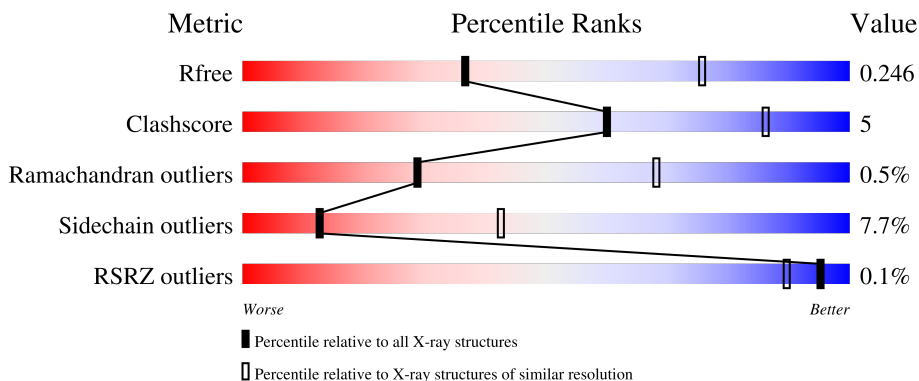
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


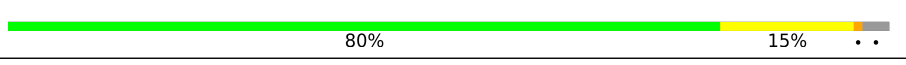
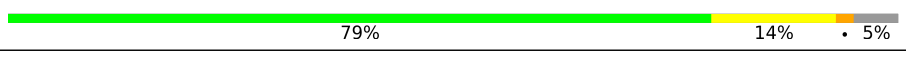
The reported resolution of this entry is 3.00 Å.

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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	 79% 15% • 5%
1	B	489	 80% 15% • •
1	C	489	 79% 14% • 5%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 11660 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
			Total	C	N	O	S			
1	A	465	3774	2439	666	649	20	0	0	0
1	B	473	3832	2471	683	658	20	0	0	0
1	C	466	3785	2445	670	650	20	0	0	0

There are 39 discrepancies between the modelled and reference sequences:

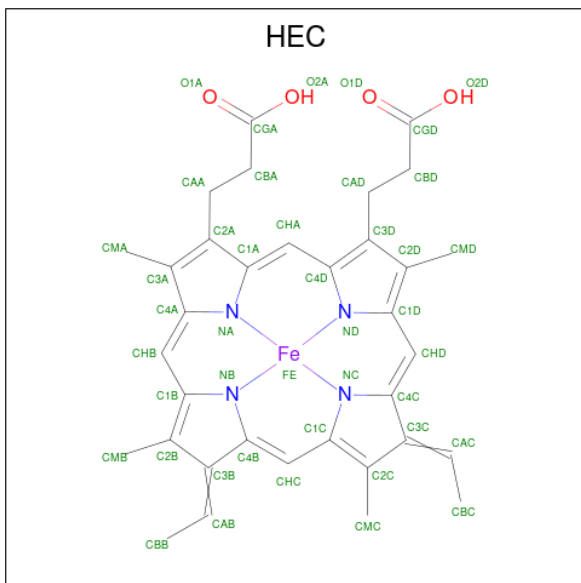
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	initiating methionine	UNP P19099
A	25	ALA	-	expression tag	UNP P19099
A	26	THR	-	expression tag	UNP P19099
A	27	LYS	-	expression tag	UNP P19099
A	504	GLY	-	expression tag	UNP P19099
A	505	GLY	-	expression tag	UNP P19099
A	506	ARG	-	expression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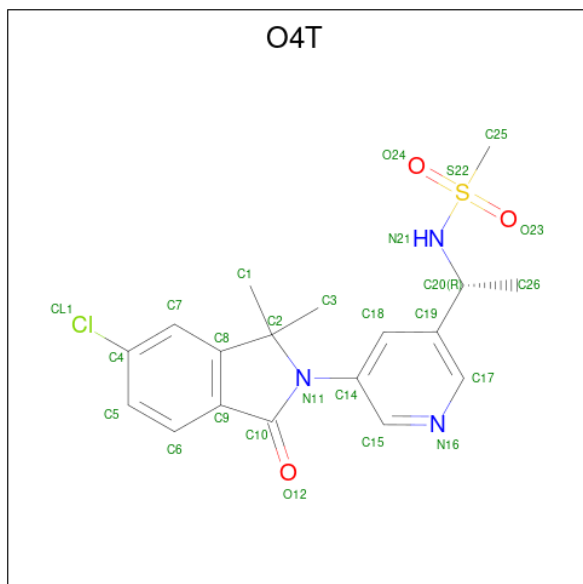
Chain	Residue	Modelled	Actual	Comment	Reference
B	510	HIS	-	expression tag	UNP P19099
B	511	HIS	-	expression tag	UNP P19099
B	512	HIS	-	expression tag	UNP P19099
C	24	MET	-	initiating methionine	UNP P19099
C	25	ALA	-	expression tag	UNP P19099
C	26	THR	-	expression tag	UNP P19099
C	27	LYS	-	expression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

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 3 is {N}-(1 {R})-1-[5-(6-chloranyl-1,1-dimethyl-3-oxidanylidene-isoindol-2-yl)pyridin-3-yl]ethyl]methanesulfonamide (three-letter code: O4T) (formula: C₁₈H₂₀ClN₃O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			S
3	A	1	Total	C	Cl	N	O	S	0	0
			26	18	1	3	3	1		
3	B	1	Total	C	Cl	N	O	S	0	0
			26	18	1	3	3	1		
3	C	1	Total	C	Cl	N	O	S	0	0
			26	18	1	3	3	1		


- Molecule 4 is water.

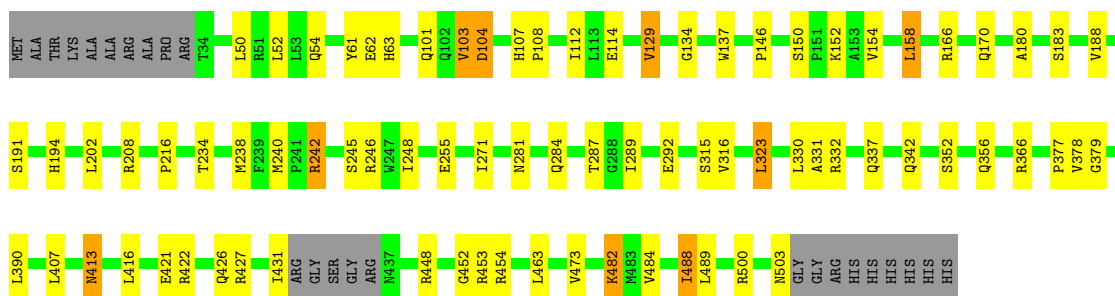
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	B	22	Total	O	0	0
			22	22		
4	C	20	Total	O	0	0
			20	20		

3 Residue-property plots


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

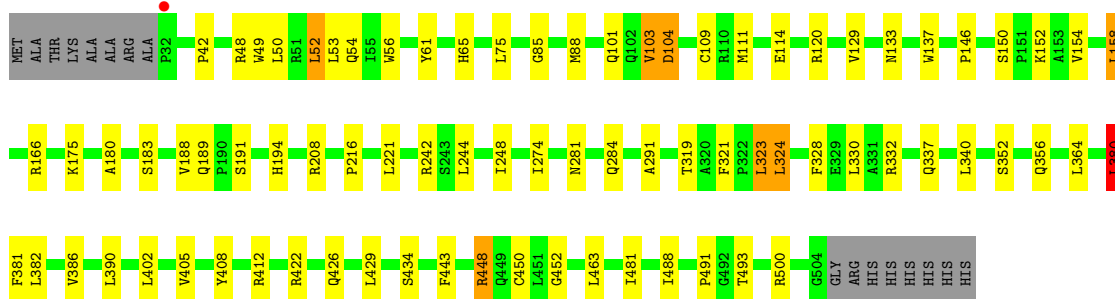
- Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain A: 




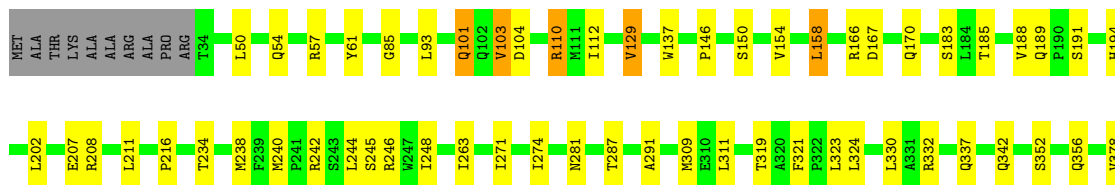
- Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain B: 



- Molecule 1: Cytochrome P450 11B2, mitochondrial

Chain C: 





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	107.32Å 121.73Å 298.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.17 – 3.00 47.17 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.17-3.00) 99.8 (47.17-3.00)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.25	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.01Å)	Xtrriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.189 , 0.221 0.211 , 0.246	Depositor DCC
R_{free} test set	1983 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	61.9	Xtrriage
Anisotropy	0.442	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11660	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: O4T, 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	0.45	0/3874	0.66	0/5257
1	B	0.44	0/3934	0.65	0/5336
1	C	0.44	0/3885	0.65	0/5271
All	All	0.45	0/11693	0.65	0/15864

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3774	0	3808	33	0
1	B	3832	0	3870	35	0
1	C	3785	0	3821	36	0
2	A	43	0	33	4	0
2	B	43	0	32	2	0
2	C	43	0	33	5	0
3	A	26	0	0	1	0
3	B	26	0	0	0	0
3	C	26	0	0	1	0
4	A	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	22	0	0	0	0
4	C	20	0	0	0	0
All	All	11660	0	11597	107	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 5.

All (107) 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:413:ASN:HD21	1:A:416:LEU:HD12	1.44	0.81
1:C:101:GLN:HG2	1:C:445:PHE:CD1	2.21	0.75
1:C:456:ALA:HB2	2:C:601:HEC:HMC2	1.74	0.70
1:C:189:GLN:HG3	1:C:324:LEU:HD22	1.74	0.69
1:C:166:ARG:HH22	1:C:352:SER:HA	1.60	0.66
1:C:321:PHE:CD2	1:C:491:PRO:HD2	2.30	0.65
1:A:166:ARG:HH22	1:A:352:SER:HA	1.61	0.64
1:C:101:GLN:HG2	1:C:445:PHE:HD1	1.65	0.61
1:B:321:PHE:CD2	1:B:491:PRO:HD2	2.35	0.61
1:B:328:PHE:CZ	1:B:332:ARG:HD2	2.35	0.61
1:C:101:GLN:HG3	1:C:438:PHE:CZ	2.37	0.59
1:B:154:VAL:O	1:B:158:LEU:HB2	2.03	0.58
2:C:601:HEC:HBB3	2:C:601:HEC:HMB1	1.86	0.57
1:A:242:ARG:O	1:A:246:ARG:HB2	2.05	0.56
1:B:166:ARG:HH12	1:B:352:SER:HA	1.69	0.56
1:C:154:VAL:O	1:C:158:LEU:HB2	2.05	0.56
1:B:244:LEU:HD22	1:B:248:ILE:HD11	1.88	0.56
1:B:481:ILE:HG23	1:B:493:THR:HG22	1.89	0.55
1:A:379:GLY:O	1:A:407:LEU:HD12	2.07	0.54
1:C:101:GLN:HG3	1:C:438:PHE:HZ	1.72	0.54
1:A:488:ILE:HG22	3:A:602:O4T:C26	2.38	0.54
1:B:330:LEU:HB3	1:B:337:GLN:HG3	1.91	0.53
1:B:65:HIS:HB3	1:B:380:LEU:HD21	1.89	0.53
1:B:189:GLN:HG3	1:B:324:LEU:CD1	2.39	0.52
1:A:103:VAL:HG21	1:A:390:LEU:HB3	1.93	0.51
1:C:330:LEU:HB3	1:C:337:GLN:HG3	1.93	0.51
1:B:323:LEU:HD22	1:B:463:LEU:HD22	1.93	0.51
1:A:234:THR:O	1:A:238:MET:HB2	2.10	0.51
1:B:408:TYR:O	1:B:412:ARG:HG2	2.10	0.50
2:C:601:HEC:HHD	2:C:601:HEC:HBC3	1.94	0.50
1:B:183:SER:HB3	1:B:500:ARG:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:THR:O	1:C:238:MET:HB2	2.12	0.49
1:A:108:PRO:HB2	1:A:448:ARG:HG3	1.94	0.49
1:A:289:ILE:O	1:A:292:GLU:HB2	2.13	0.49
1:A:330:LEU:HB3	1:A:337:GLN:HG3	1.93	0.49
2:C:601:HEC:HMB1	2:C:601:HEC:CBB	2.43	0.49
1:A:183:SER:HB3	1:A:500:ARG:HA	1.95	0.48
1:C:311:LEU:HA	2:C:601:HEC:CBC	2.43	0.48
1:B:137:TRP:CZ2	1:B:448:ARG:HG2	2.49	0.48
1:A:146:PRO:HA	1:A:150:SER:HB3	1.95	0.48
2:B:601:HEC:HMB1	2:B:601:HEC:HBB2	1.96	0.48
1:B:103:VAL:HG21	1:B:390:LEU:HB3	1.95	0.48
1:A:240:MET:HG3	1:A:245:SER:HB3	1.96	0.47
1:C:263:ILE:HG22	1:C:309:MET:HE2	1.95	0.47
1:C:146:PRO:HA	1:C:150:SER:HB3	1.96	0.47
1:A:154:VAL:HG12	1:A:158:LEU:HD12	1.95	0.47
1:C:194:HIS:NE2	1:C:216:PRO:HB3	2.29	0.47
1:C:245:SER:HA	1:C:248:ILE:HG22	1.96	0.47
1:A:194:HIS:NE2	1:A:216:PRO:HB3	2.30	0.47
1:C:103:VAL:HG21	1:C:390:LEU:HB3	1.96	0.47
1:B:111:MET:HG2	1:B:402:LEU:HD13	1.96	0.47
1:A:427:ARG:O	1:A:431:ILE:HG12	2.15	0.47
1:C:488:ILE:HG22	3:C:602:O4T:C26	2.45	0.47
1:C:183:SER:HB3	1:C:500:ARG:HA	1.95	0.46
1:B:382:LEU:HD12	1:B:405:VAL:HB	1.97	0.46
1:B:194:HIS:NE2	1:B:216:PRO:HB3	2.29	0.46
1:A:315:SER:HA	2:A:601:HEC:CMC	2.46	0.46
1:A:315:SER:HA	2:A:601:HEC:HMC3	1.98	0.46
1:B:146:PRO:HA	1:B:150:SER:HB3	1.98	0.46
1:A:62:GLU:HB3	1:A:484:VAL:HG22	1.98	0.46
1:A:331:ALA:HB2	1:A:473:VAL:HG12	1.97	0.46
1:A:154:VAL:O	1:A:158:LEU:HB2	2.17	0.45
1:A:180:ALA:HB1	1:C:287:THR:HG22	1.99	0.45
1:B:452:GLY:HA3	2:B:601:HEC:HBC2	1.98	0.45
1:C:263:ILE:HG22	1:C:309:MET:CE	2.46	0.45
1:A:52:LEU:HD21	1:A:240:MET:HE3	1.98	0.45
1:B:323:LEU:CD2	1:B:463:LEU:HD22	2.47	0.45
1:C:101:GLN:O	1:C:104:ASP:HB2	2.16	0.45
1:A:287:THR:HG22	1:B:180:ALA:HB1	1.99	0.45
1:B:88:MET:HG3	1:B:402:LEU:HD23	1.99	0.45
1:B:101:GLN:O	1:B:104:ASP:HB2	2.17	0.44
1:B:381:PHE:HA	1:B:405:VAL:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:TRP:CD1	1:B:248:ILE:HG22	2.52	0.44
1:C:382:LEU:HB2	1:C:405:VAL:HB	2.00	0.44
1:A:452:GLY:HA3	2:A:601:HEC:HBC2	2.01	0.43
1:B:244:LEU:O	1:B:248:ILE:HG13	2.18	0.43
1:A:453:ARG:HH22	1:A:454:ARG:HH21	1.66	0.43
1:C:424:ASN:O	1:C:427:ARG:HG2	2.17	0.43
1:B:328:PHE:CE2	1:B:332:ARG:HD2	2.53	0.43
1:A:377:PRO:O	1:A:489:LEU:HB3	2.18	0.43
1:C:240:MET:HG3	1:C:245:SER:HB3	2.01	0.43
1:C:129:VAL:HG22	1:C:137:TRP:CD1	2.54	0.42
1:B:208:ARG:HA	1:B:208:ARG:HD2	1.79	0.42
1:B:42:PRO:HB3	1:B:75:LEU:HD22	2.01	0.42
1:A:208:ARG:HA	1:A:208:ARG:HD2	1.80	0.42
1:C:274:ILE:HD11	1:C:291:ALA:HB2	2.01	0.42
1:C:167:ASP:HA	1:C:170:GLN:HG2	2.01	0.42
1:C:413:ASN:OD1	1:C:416:LEU:HG	2.20	0.42
1:A:323:LEU:HD22	1:A:463:LEU:HD22	2.02	0.42
1:B:49:TRP:O	1:B:53:LEU:HG	2.19	0.42
1:C:208:ARG:HA	1:C:208:ARG:HD2	1.80	0.41
1:C:110:ARG:HG2	1:C:383:GLU:HG2	2.01	0.41
1:C:443:PHE:HB3	1:C:450:CYS:HB3	2.02	0.41
1:B:274:ILE:HD11	1:B:291:ALA:HB2	2.02	0.41
1:C:488:ILE:H	1:C:488:ILE:HG13	1.67	0.41
1:A:63:HIS:CD2	1:A:482:LYS:HZ1	2.39	0.41
1:C:194:HIS:HD2	1:C:211:LEU:HD22	1.86	0.41
2:A:601:HEC:HBB3	2:A:601:HEC:HMB1	2.03	0.41
1:B:340:LEU:HD23	1:B:364:LEU:HB3	2.03	0.41
1:B:49:TRP:HA	1:B:52:LEU:HD23	2.02	0.41
1:B:443:PHE:HB3	1:B:450:CYS:HB3	2.01	0.41
1:A:107:HIS:HB3	1:A:134:GLY:HA2	2.03	0.41
1:C:185:THR:HG22	1:C:496:LEU:HG	2.02	0.41
1:A:202:LEU:HD22	1:A:208:ARG:HD3	2.02	0.40
1:A:129:VAL:HG22	1:A:137:TRP:CD1	2.55	0.40
1:B:109:CYS:HB2	1:B:133:ASN:OD1	2.22	0.40
1:C:202:LEU:HD22	1:C:208:ARG:HD3	2.03	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	461/489 (94%)	447 (97%)	12 (3%)	2 (0%)	34	72
1	B	471/489 (96%)	453 (96%)	15 (3%)	3 (1%)	25	64
1	C	462/489 (94%)	443 (96%)	17 (4%)	2 (0%)	34	72
All	All	1394/1467 (95%)	1343 (96%)	44 (3%)	7 (0%)	29	68

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	431	ILE
1	A	104	ASP
1	B	380	LEU
1	B	386	VAL
1	A	316	VAL
1	B	85	GLY
1	C	85	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	410/426 (96%)	377 (92%)	33 (8%)	12	40
1	B	415/426 (97%)	385 (93%)	30 (7%)	14	45
1	C	411/426 (96%)	379 (92%)	32 (8%)	12	42
All	All	1236/1278 (97%)	1141 (92%)	95 (8%)	13	42

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LEU
1	A	54	GLN
1	A	61	TYR
1	A	101	GLN
1	A	103	VAL
1	A	104	ASP
1	A	112	ILE
1	A	114	GLU
1	A	129	VAL
1	A	152	LYS
1	A	158	LEU
1	A	170	GLN
1	A	188	VAL
1	A	191	SER
1	A	242	ARG
1	A	248	ILE
1	A	255	GLU
1	A	271	ILE
1	A	281	ASN
1	A	284	GLN
1	A	323	LEU
1	A	332	ARG
1	A	342	GLN
1	A	356	GLN
1	A	366	ARG
1	A	378	VAL
1	A	413	ASN
1	A	421	GLU
1	A	422	ARG
1	A	426	GLN
1	A	482	LYS
1	A	488	ILE
1	A	503	ASN
1	B	48	ARG
1	B	50	LEU
1	B	52	LEU
1	B	54	GLN
1	B	61	TYR
1	B	103	VAL
1	B	104	ASP
1	B	114	GLU
1	B	120	ARG

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Mol	Chain	Res	Type
1	B	129	VAL
1	B	152	LYS
1	B	158	LEU
1	B	175	LYS
1	B	188	VAL
1	B	191	SER
1	B	221	LEU
1	B	242	ARG
1	B	281	ASN
1	B	284	GLN
1	B	319	THR
1	B	323	LEU
1	B	324	LEU
1	B	356	GLN
1	B	380	LEU
1	B	422	ARG
1	B	426	GLN
1	B	429	LEU
1	B	434	SER
1	B	448	ARG
1	B	488	ILE
1	C	50	LEU
1	C	54	GLN
1	C	57	ARG
1	C	61	TYR
1	C	93	LEU
1	C	101	GLN
1	C	103	VAL
1	C	110	ARG
1	C	112	ILE
1	C	129	VAL
1	C	158	LEU
1	C	188	VAL
1	C	191	SER
1	C	207	GLU
1	C	242	ARG
1	C	244	LEU
1	C	246	ARG
1	C	271	ILE
1	C	281	ASN
1	C	319	THR
1	C	323	LEU

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Mol	Chain	Res	Type
1	C	332	ARG
1	C	342	GLN
1	C	356	GLN
1	C	378	VAL
1	C	380	LEU
1	C	383	GLU
1	C	416	LEU
1	C	422	ARG
1	C	427	ARG
1	C	480	ASP
1	C	488	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	GLN
1	A	342	GLN
1	A	394	ASN
1	A	413	ASN
1	B	54	GLN
1	B	107	HIS
1	B	178	GLN
1	B	222	ASN
1	B	404	GLN
1	C	342	GLN
1	C	437	ASN
1	C	478	GLN

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

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	O4T	B	602	2	27,28,28	1.04	2 (7%)	39,44,44	3.09	18 (46%)
2	HEC	A	601	1,3	32,50,50	1.90	7 (21%)	24,82,82	1.83	8 (33%)
2	HEC	B	601	1,3	32,50,50	1.99	7 (21%)	24,82,82	1.52	6 (25%)
3	O4T	C	602	2	27,28,28	1.05	1 (3%)	39,44,44	2.42	12 (30%)
3	O4T	A	602	2	27,28,28	1.06	2 (7%)	39,44,44	2.25	14 (35%)
2	HEC	C	601	1,3	32,50,50	1.89	6 (18%)	24,82,82	1.58	6 (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
3	O4T	B	602	2	-	5/13/33/33	0/3/3/3
2	HEC	A	601	1,3	-	3/10/54/54	-
2	HEC	B	601	1,3	-	2/10/54/54	-
3	O4T	C	602	2	-	0/13/33/33	0/3/3/3
3	O4T	A	602	2	-	0/13/33/33	0/3/3/3
2	HEC	C	601	1,3	-	2/10/54/54	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEC	C3C-C2C	-5.58	1.34	1.40
2	A	601	HEC	CBC-CAC	-5.01	1.30	1.49
2	B	601	HEC	CBB-CAB	-4.84	1.31	1.49
2	C	601	HEC	CBC-CAC	-4.83	1.31	1.49
2	B	601	HEC	C3C-C2C	-4.62	1.35	1.40
2	C	601	HEC	CBB-CAB	-4.41	1.32	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	HEC	C3C-C2C	-4.05	1.36	1.40
2	B	601	HEC	CBC-CAC	-4.00	1.34	1.49
2	B	601	HEC	C2B-C3B	-3.93	1.36	1.40
2	C	601	HEC	C4B-C3B	3.63	1.49	1.43
2	A	601	HEC	C4B-C3B	3.56	1.49	1.43
2	B	601	HEC	C4B-C3B	3.42	1.49	1.43
2	A	601	HEC	CBB-CAB	-3.38	1.36	1.49
2	C	601	HEC	C2B-C3B	-3.35	1.37	1.40
2	B	601	HEC	CAD-C3D	-3.08	1.47	1.52
3	B	602	O4T	C25-S22	2.99	1.82	1.75
2	B	601	HEC	C3D-C2D	-2.92	1.29	1.37
3	A	602	O4T	C25-S22	2.76	1.81	1.75
3	C	602	O4T	C25-S22	2.71	1.81	1.75
2	A	601	HEC	CAD-C3D	-2.59	1.48	1.52
3	A	602	O4T	S22-N21	2.51	1.67	1.62
3	B	602	O4T	S22-N21	2.39	1.67	1.62
2	A	601	HEC	O2A-CGA	2.35	1.38	1.30
2	C	601	HEC	CAA-C2A	-2.27	1.48	1.52
2	A	601	HEC	C1C-NC	2.20	1.40	1.36

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	O4T	C8-C2-N11	10.59	106.50	101.39
3	B	602	O4T	C9-C10-N11	7.09	110.65	106.16
3	C	602	O4T	C9-C10-N11	6.63	110.37	106.16
3	B	602	O4T	C2-N11-C10	-6.49	108.06	112.94
3	C	602	O4T	C8-C2-N11	6.35	104.45	101.39
3	A	602	O4T	C8-C2-N11	6.00	104.28	101.39
3	A	602	O4T	C9-C10-N11	5.13	109.41	106.16
3	B	602	O4T	C2-C8-C9	-4.87	107.16	110.19
3	C	602	O4T	C2-N11-C10	-4.50	109.56	112.94
3	C	602	O4T	C7-C8-C2	4.29	133.17	126.46
3	B	602	O4T	C15-C14-N11	4.14	124.44	119.84
3	B	602	O4T	C25-S22-N21	-4.05	99.52	107.13
3	A	602	O4T	C2-N11-C10	-3.95	109.97	112.94
3	C	602	O4T	C2-C8-C9	-3.83	107.81	110.19
3	C	602	O4T	O23-S22-N21	-3.75	101.50	107.23
3	B	602	O4T	C17-N16-C15	3.71	122.54	117.48
3	B	602	O4T	C7-C8-C2	3.60	132.09	126.46
2	C	601	HEC	CBA-CAA-C2A	-3.40	106.87	112.60
2	A	601	HEC	C1D-C2D-C3D	-3.31	104.69	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	HEC	CMB-C2B-C3B	3.29	129.69	125.82
3	A	602	O4T	C26-C20-N21	3.26	113.97	108.36
3	A	602	O4T	C7-C8-C2	3.26	131.56	126.46
3	A	602	O4T	C14-C15-N16	-3.13	119.46	122.92
3	B	602	O4T	C14-C15-N16	-3.08	119.51	122.92
3	A	602	O4T	C2-C8-C9	-3.07	108.28	110.19
3	C	602	O4T	C3-C2-N11	3.06	115.34	111.46
2	A	601	HEC	O2A-CGA-CBA	2.88	123.30	114.03
2	A	601	HEC	CMD-C2D-C3D	2.87	130.35	124.94
3	C	602	O4T	C1-C2-N11	-2.86	107.83	111.46
2	B	601	HEC	CMC-C2C-C3C	2.85	129.17	125.82
2	A	601	HEC	O2D-CGD-O1D	-2.82	116.26	123.30
3	A	602	O4T	C3-C2-N11	2.81	115.02	111.46
3	C	602	O4T	O12-C10-C9	-2.79	123.24	128.68
3	C	602	O4T	C14-C15-N16	-2.71	119.92	122.92
2	A	601	HEC	CMB-C2B-C3B	2.70	129.00	125.82
3	C	602	O4T	C17-N16-C15	2.70	121.16	117.48
3	A	602	O4T	C17-N16-C15	2.69	121.15	117.48
3	A	602	O4T	C7-C4-CL1	-2.65	115.83	119.15
3	B	602	O4T	O12-C10-C9	-2.62	123.58	128.68
3	A	602	O4T	O12-C10-C9	-2.60	123.62	128.68
3	A	602	O4T	O23-S22-N21	-2.59	103.27	107.23
3	A	602	O4T	C14-N11-C10	2.58	125.26	123.46
3	A	602	O4T	C5-C4-CL1	2.55	123.35	119.35
3	B	602	O4T	O24-S22-C25	2.52	112.32	108.28
2	B	601	HEC	CMC-C2C-C1C	-2.51	124.61	128.46
3	B	602	O4T	C14-N11-C10	2.48	125.19	123.46
2	A	601	HEC	O2D-CGD-CBD	2.38	121.67	114.03
2	C	601	HEC	CMB-C2B-C1B	-2.34	124.87	128.46
3	B	602	O4T	C3-C2-C8	-2.32	108.50	112.16
2	B	601	HEC	CMB-C2B-C1B	-2.30	124.94	128.46
2	A	601	HEC	CMD-C2D-C1D	-2.29	124.94	128.46
2	C	601	HEC	CMB-C2B-C3B	2.17	128.37	125.82
2	C	601	HEC	C4C-C3C-C2C	2.17	108.69	106.35
3	B	602	O4T	C1-C2-C8	-2.16	108.76	112.16
3	B	602	O4T	C5-C4-CL1	2.16	122.72	119.35
2	C	601	HEC	CMA-C3A-C2A	2.14	128.97	124.94
2	B	601	HEC	O2D-CGD-O1D	-2.12	118.01	123.30
2	C	601	HEC	CMD-C2D-C1D	-2.09	125.25	128.46
3	B	602	O4T	C7-C4-CL1	-2.09	116.54	119.15
2	A	601	HEC	O1A-CGA-CBA	-2.06	116.45	123.08
3	B	602	O4T	C1-C2-N11	-2.05	108.86	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	O4T	C18-C14-N11	-2.04	117.12	119.62
2	B	601	HEC	CAD-CBD-CGD	-2.03	108.07	113.76
3	C	602	O4T	C3-C2-C8	-2.02	108.97	112.16

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	O4T	C20-N21-S22-O23
3	B	602	O4T	C20-N21-S22-C25
2	A	601	HEC	C2A-CAA-CBA-CGA
3	B	602	O4T	C26-C20-N21-S22
2	B	601	HEC	CAD-CBD-CGD-O1D
3	B	602	O4T	C17-C19-C20-C26
2	B	601	HEC	CAD-CBD-CGD-O2D
2	C	601	HEC	CAD-CBD-CGD-O1D
3	B	602	O4T	C18-C19-C20-C26
2	C	601	HEC	CAD-CBD-CGD-O2D
2	A	601	HEC	CAD-CBD-CGD-O1D
2	A	601	HEC	CAD-CBD-CGD-O2D

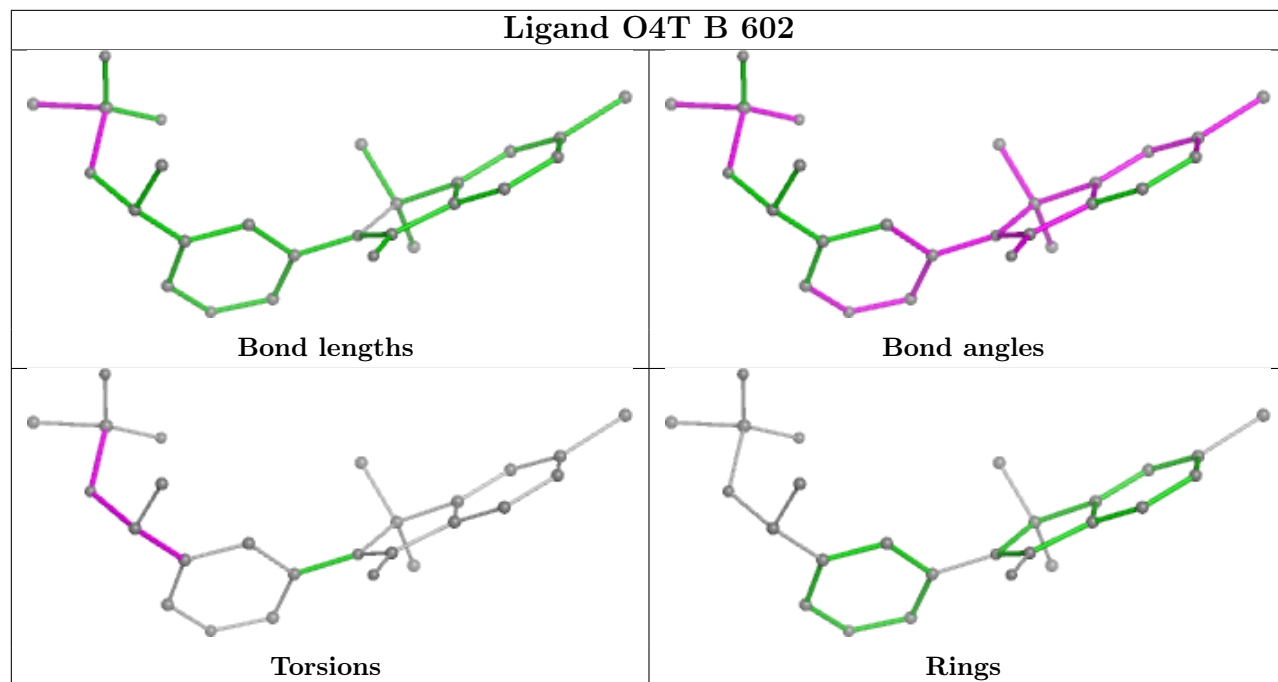
There are no ring outliers.

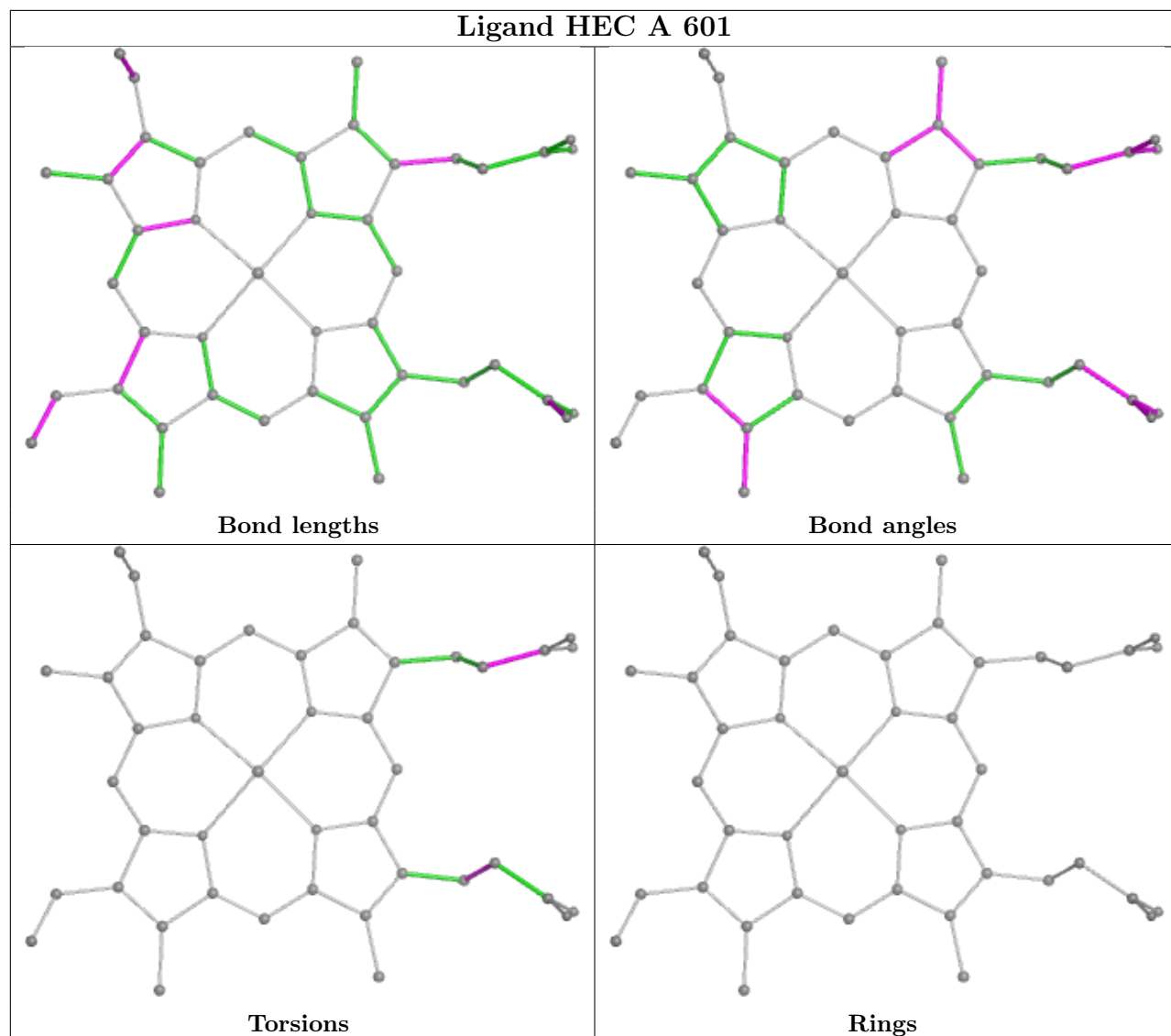
5 monomers are involved in 13 short contacts:

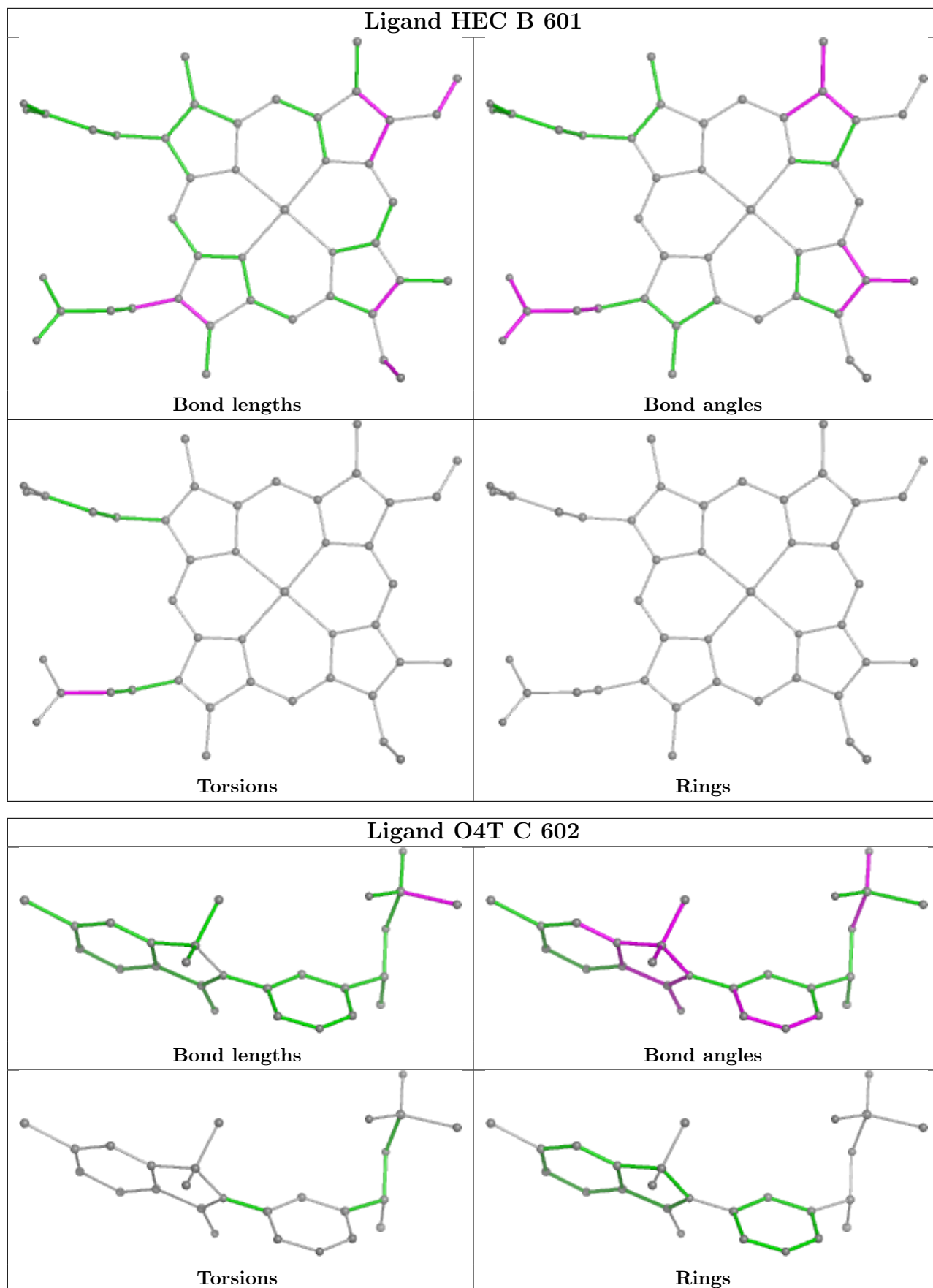
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEC	4	0
2	B	601	HEC	2	0
3	C	602	O4T	1	0
3	A	602	O4T	1	0
2	C	601	HEC	5	0

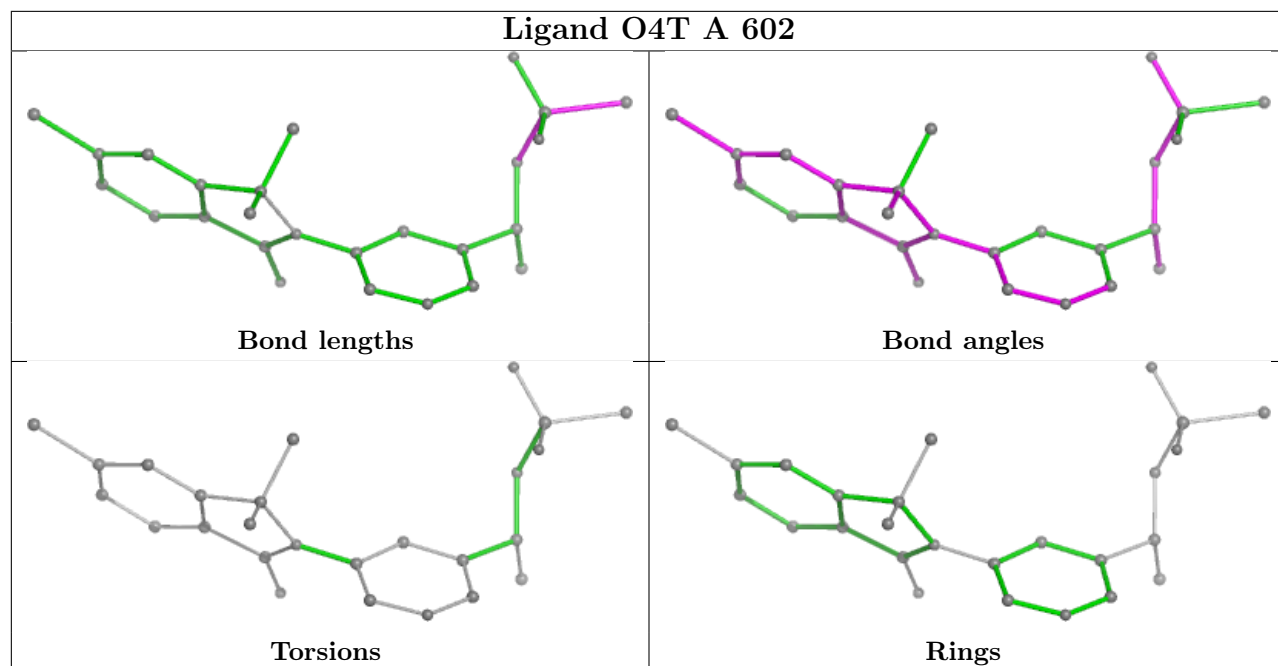
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

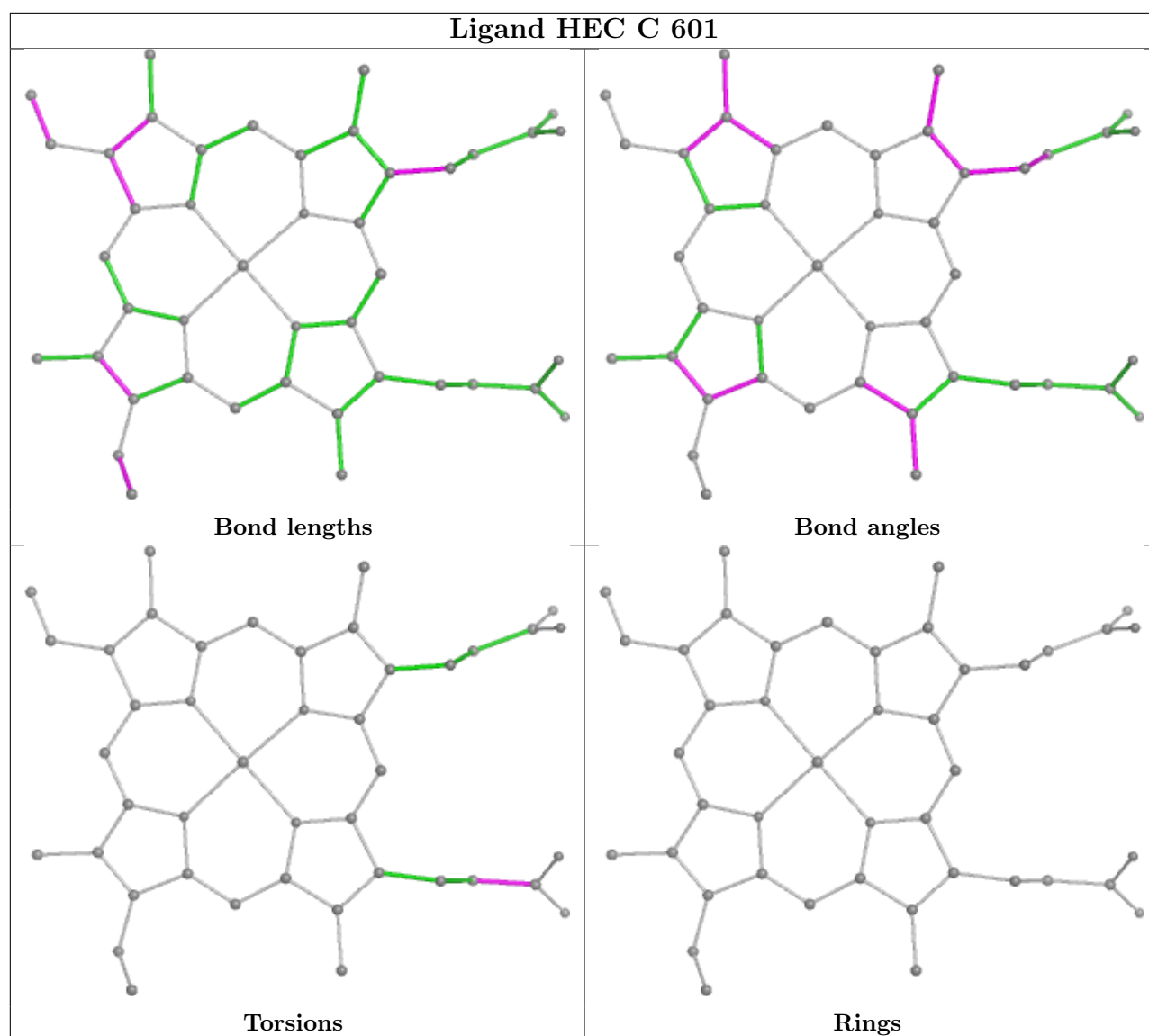
equivalents in the CSD to analyse the geometry.











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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	465/489 (95%)	-0.38	0 100 100	42, 61, 86, 115	0
1	B	473/489 (96%)	-0.37	1 (0%) 95 87	45, 63, 88, 122	0
1	C	466/489 (95%)	-0.40	0 100 100	40, 64, 90, 127	0
All	All	1404/1467 (95%)	-0.38	1 (0%) 95 89	40, 63, 88, 127	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	PRO	3.0

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 monosaccharides 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.

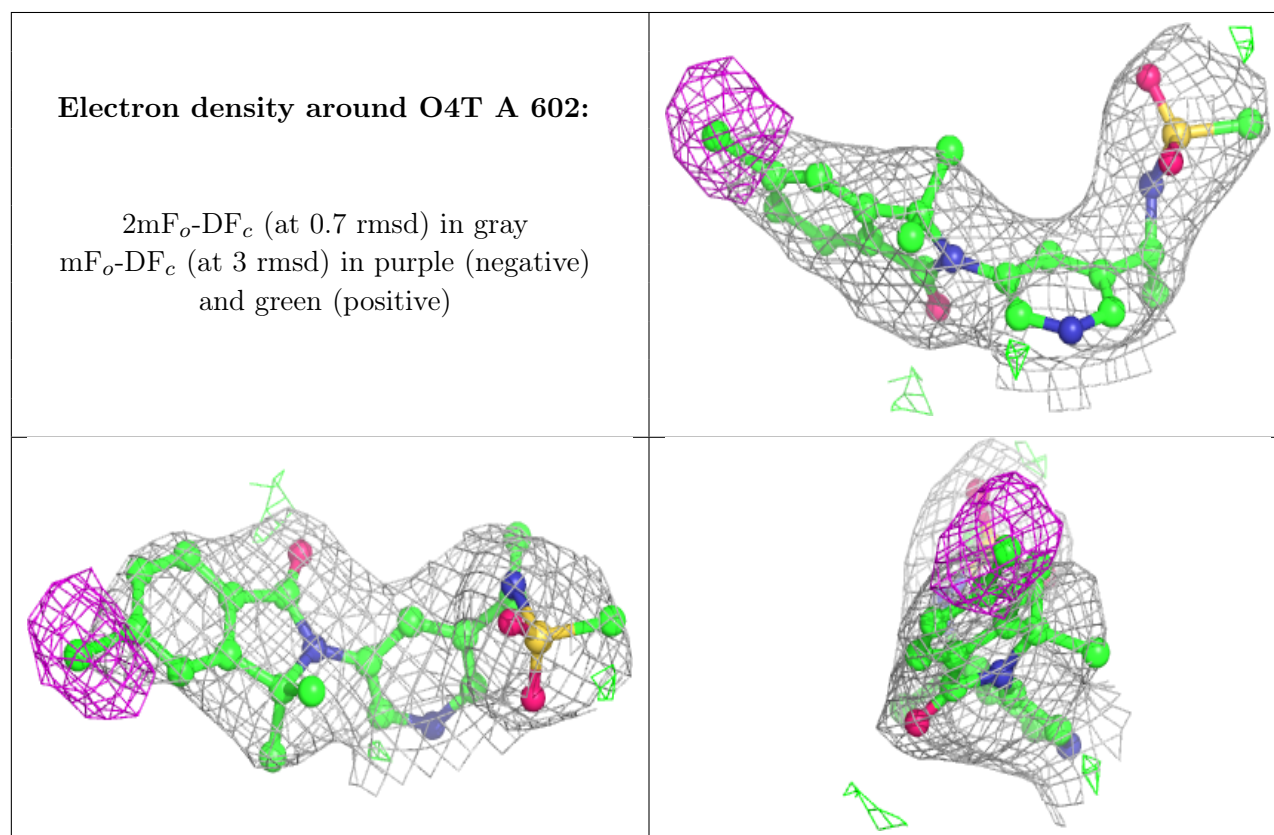
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	O4T	A	602	26/26	0.95	0.23	45,59,70,89	0
3	O4T	B	602	26/26	0.95	0.23	47,59,73,93	0

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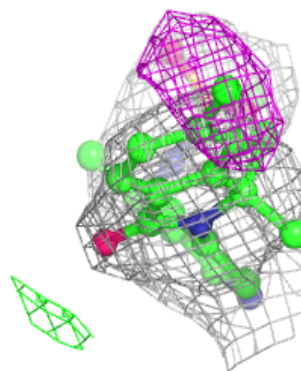
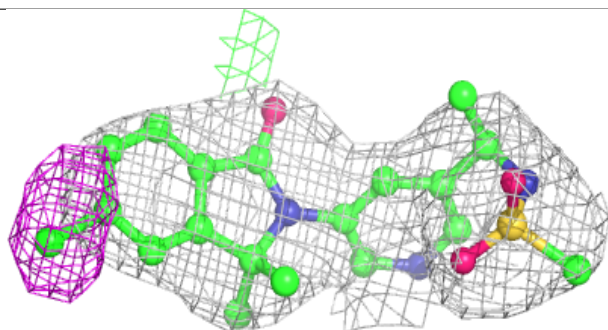
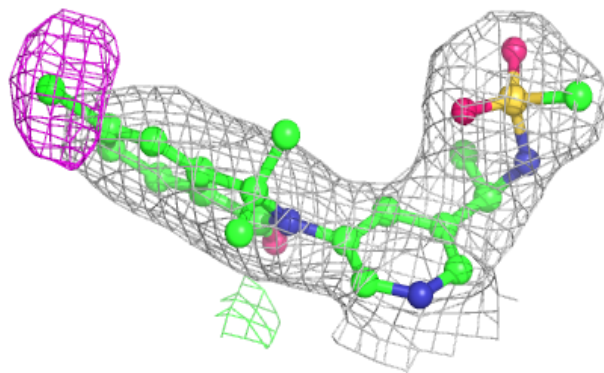
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	O4T	C	602	26/26	0.95	0.20	51,57,69,88	0
2	HEC	A	601	43/43	0.98	0.17	44,45,51,58	0
2	HEC	B	601	43/43	0.98	0.18	50,52,56,57	0
2	HEC	C	601	43/43	0.98	0.16	44,45,50,50	0

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.

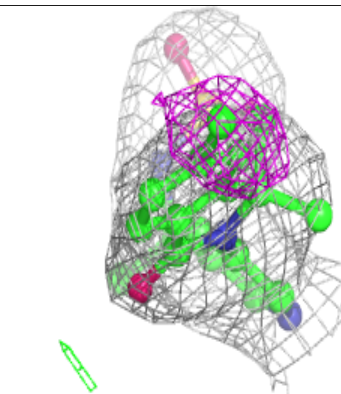
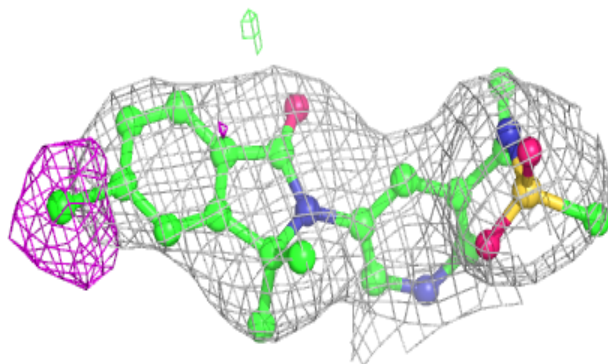
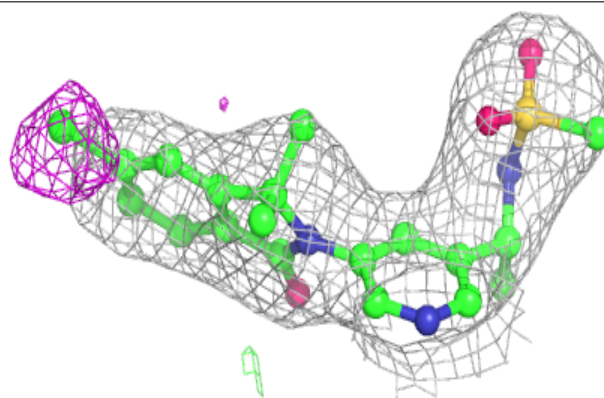


Electron density around O4T B 602:

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

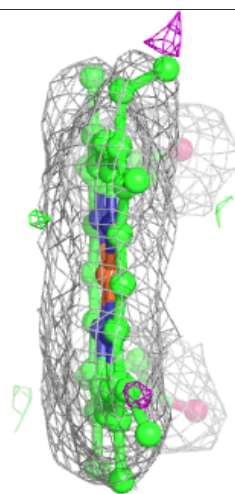
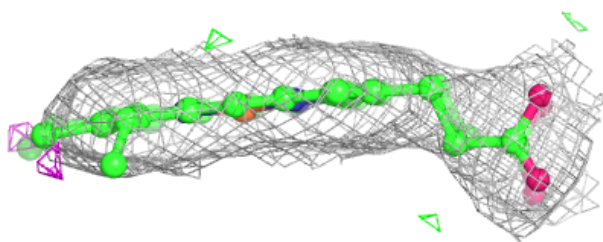
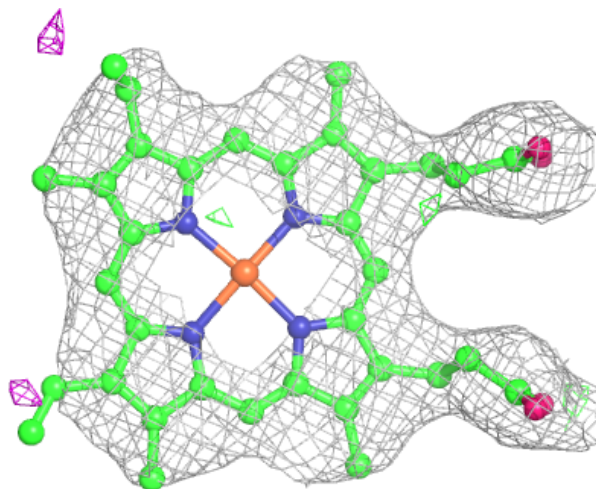
**Electron density around O4T C 602:**

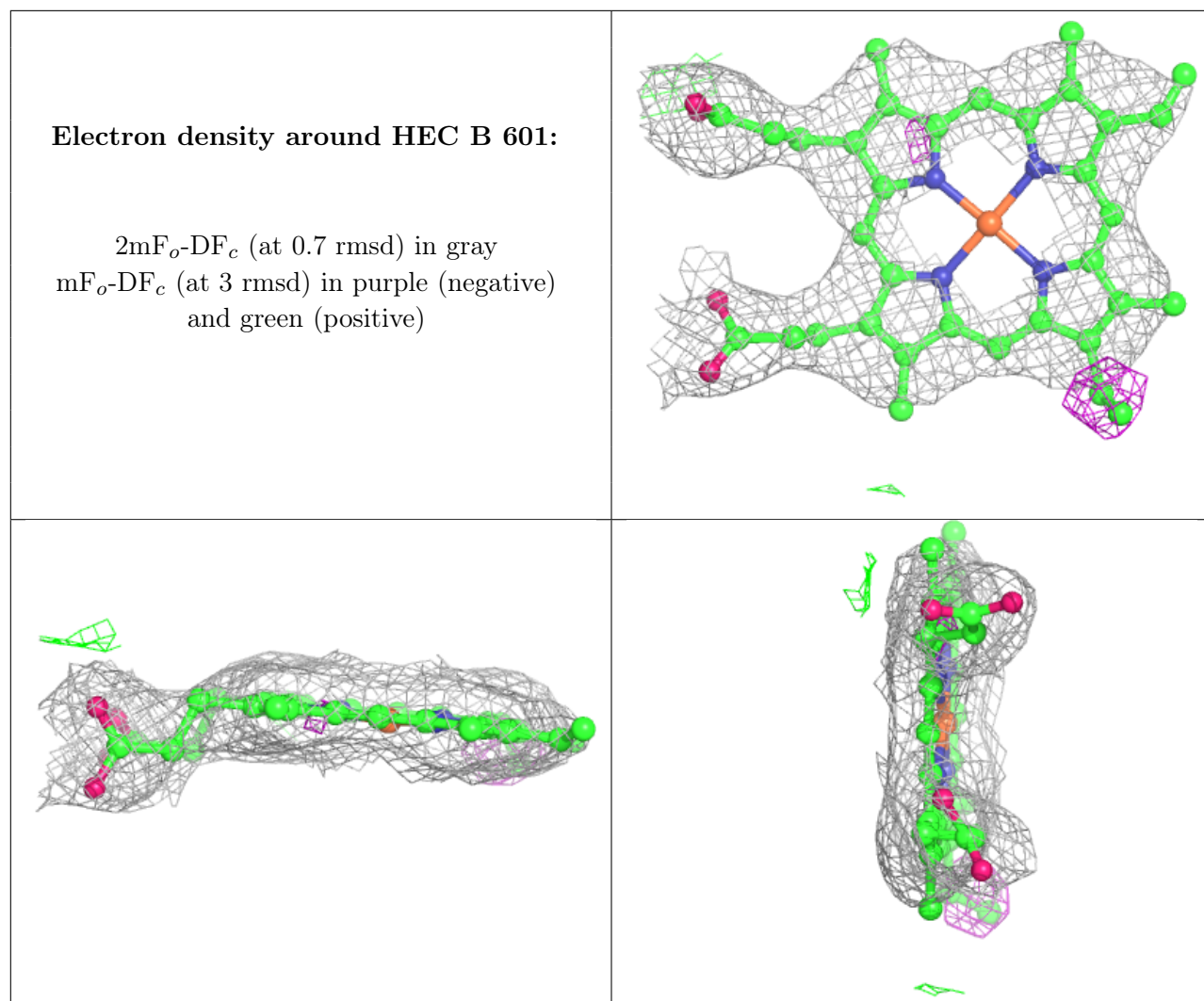
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

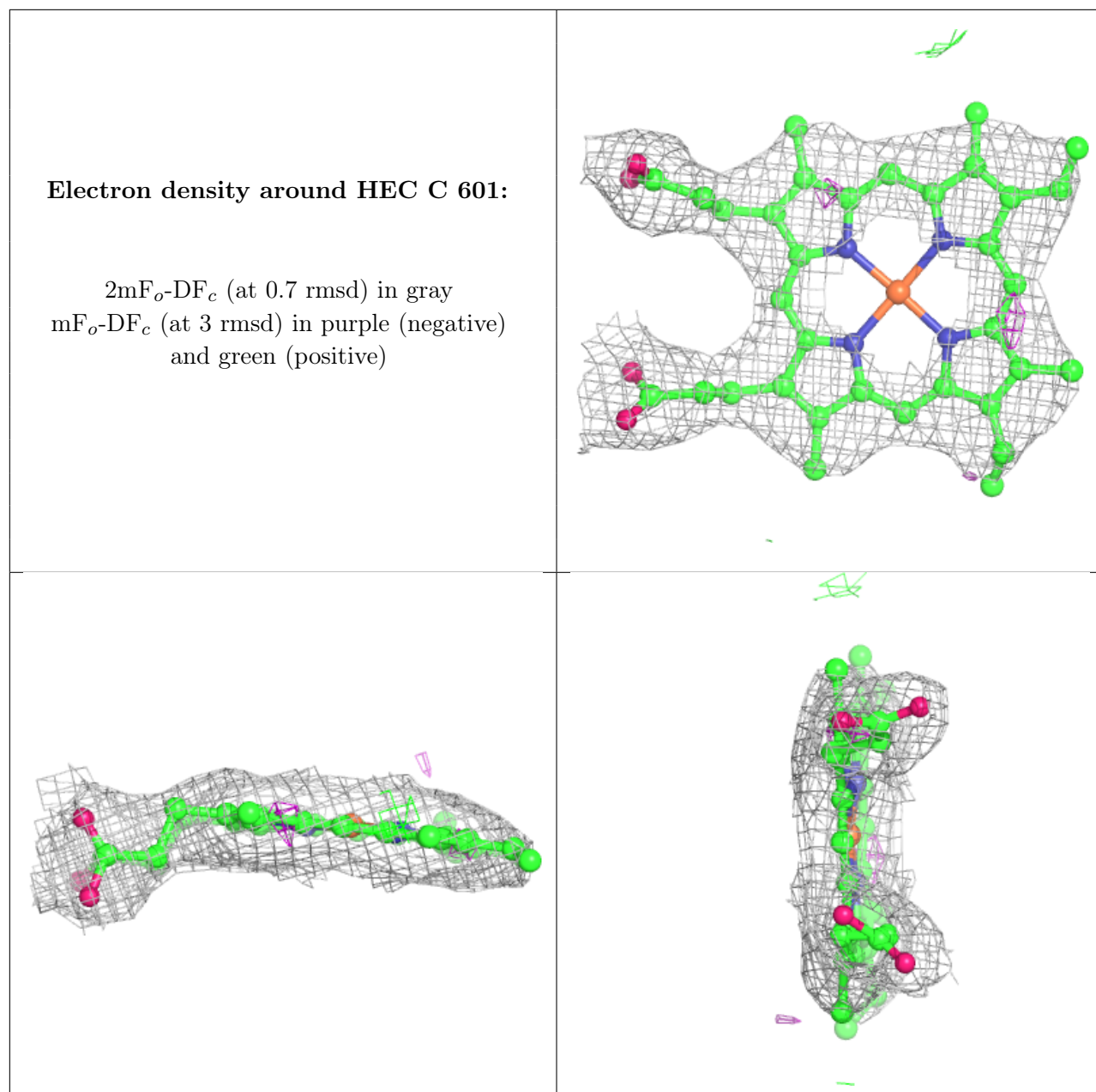


Electron density around HEC A 601:

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







6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.