



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 2, 2021 – 01:14 pm GMT

PDB ID : 6ZBO
Title : HIF Prolyl Hydroxylase 2 (PHD2/EGLN1) in Complex with 1-(6-morpholino pyrimidin-4-yl)-4-(1H-1,2,3-triazol-1-yl)-1H-pyrazol-5-ol (Molidustat)
Authors : Figg Jr, W.D.; McDonough, M.A.; Nakashima, Y.; Holt-Martyn, J.P.; Schofield, C.J.
Deposited on : 2020-06-08
Resolution : 1.79 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

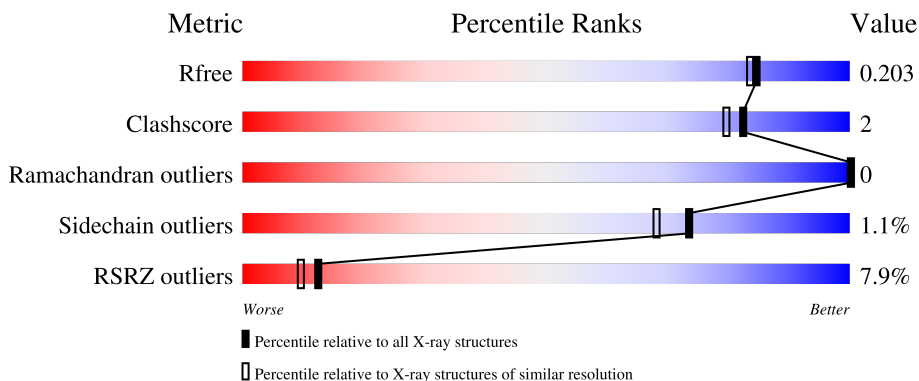
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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.



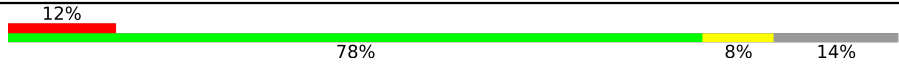
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	227	 5% 84% 6% 10%
1	B	227	 4% 85% 5% 10%
1	C	227	 5% 84% 5% 11%
1	D	227	 6% 86% 5% 11%
1	E	227	 10% 78% 8% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	227	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '12%', a large green segment labeled '78%', a yellow segment labeled '8%', and a grey segment on the right labeled '14%'.</p>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19772 atoms, of which 9394 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.

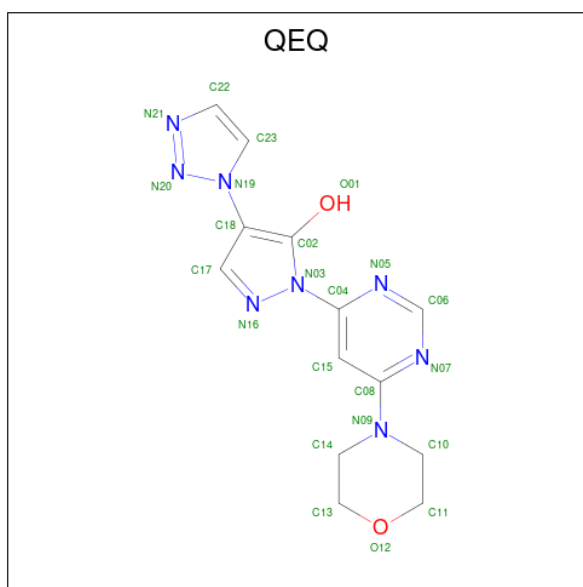
- Molecule 1 is a protein called Egl nine homolog 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	204	3172	1032	1552	277	299	12	0	4	0
1	B	205	3189	1031	1567	278	301	12	0	4	0
1	C	202	3186	1026	1571	281	296	12	0	4	0
1	D	202	3170	1021	1568	279	290	12	0	3	0
1	E	197	3115	1000	1540	277	286	12	0	4	0
1	F	196	3074	994	1512	271	285	12	0	4	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		

- Molecule 3 is 2-(6-morpholin-4-ylpyrimidin-4-yl)-4-(1,2,3-triazol-1-yl)pyrazol-3-ol (three-letter code: QEQ) (formula: C₁₃H₁₄N₈O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
3	A	1	Total 37	C 13	H 14	N 8	O 2	0	0
3	B	1	Total 37	C 13	H 14	N 8	O 2	0	0
3	C	1	Total 37	C 13	H 14	N 8	O 2	0	0
3	D	1	Total 37	C 13	H 14	N 8	O 2	0	0
3	E	1	Total 37	C 13	H 14	N 8	O 2	0	0
3	F	1	Total 37	C 13	H 14	N 8	O 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	3	Total 3	Cl 3	0	0
4	B	2	Total 2	Cl 2	0	0
4	C	1	Total 1	Cl 1	0	0
4	D	2	Total 2	Cl 2	0	0
4	E	2	Total 2	Cl 2	0	0
4	F	3	Total 3	Cl 3	0	0

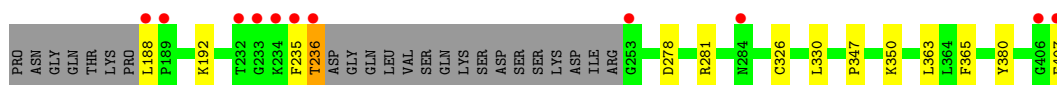
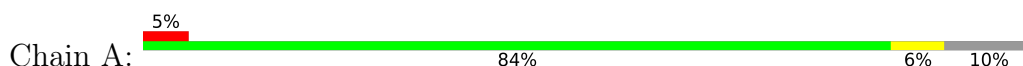
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	139	Total 141	O 141	0	3
5	B	125	Total 125	O 125	0	0
5	C	95	Total 96	O 96	0	1
5	D	102	Total 102	O 102	0	0
5	E	70	Total 70	O 70	0	1
5	F	91	Total 91	O 91	0	0

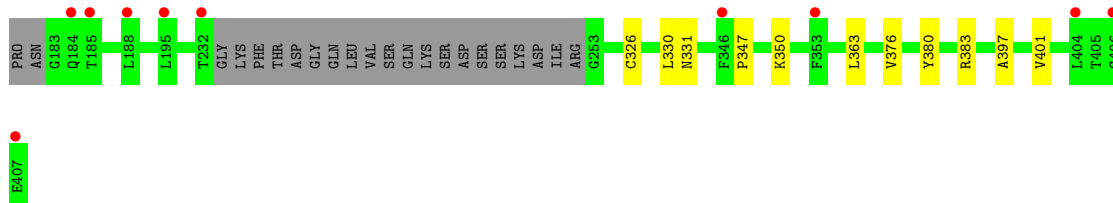
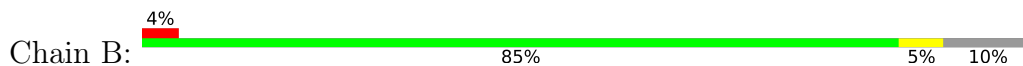
3 Residue-property plots [i](#)

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.

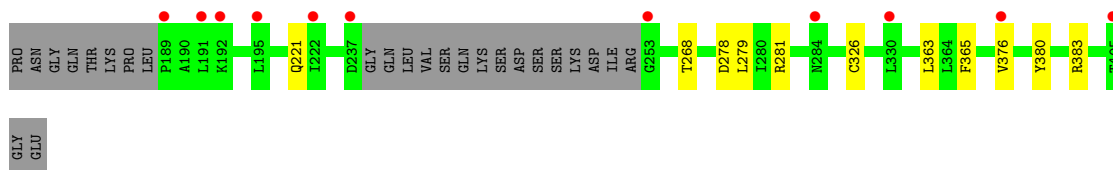
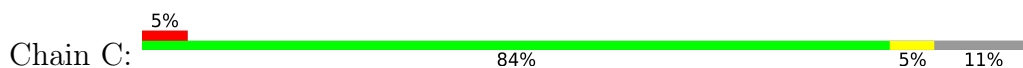
- Molecule 1: Egl nine homolog 1



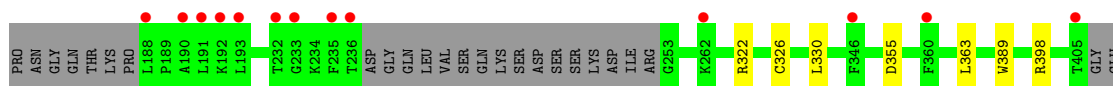
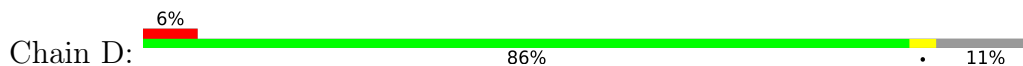
- Molecule 1: Egl nine homolog 1



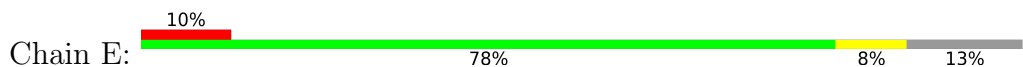
- Molecule 1: Egl nine homolog 1

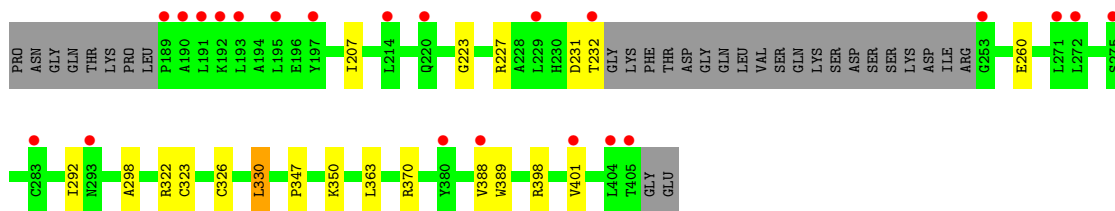


- Molecule 1: Egl nine homolog 1

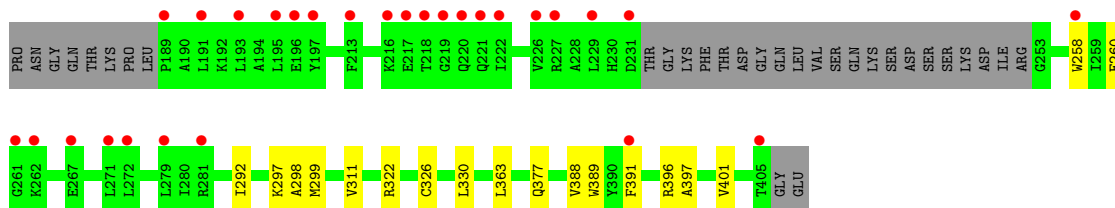
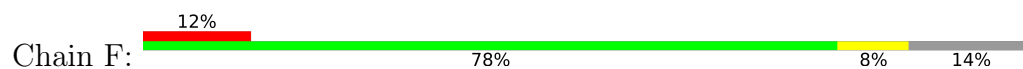


- Molecule 1: Egl nine homolog 1





- Molecule 1: Egl nine homolog 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.12Å 75.15Å 127.22Å 90.00° 95.31° 90.00°	Depositor
Resolution (Å)	53.71 – 1.79 53.71 – 1.79	Depositor EDS
% Data completeness (in resolution range)	98.2 (53.71-1.79) 98.2 (53.71-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.80Å)	Xtrriage
Refinement program	PHENIX 1.19.1	Depositor
R, R_{free}	0.180 , 0.206 0.178 , 0.203	Depositor DCC
R_{free} test set	6820 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtrriage
Anisotropy	0.497	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19772	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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: QEQ, MN, CL

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	0.42	0/1661	0.60	0/2251
1	B	0.39	0/1668	0.57	0/2257
1	C	0.38	0/1661	0.58	0/2245
1	D	0.33	0/1648	0.55	0/2227
1	E	0.34	0/1623	0.56	0/2193
1	F	0.35	0/1607	0.57	0/2173
All	All	0.37	0/9868	0.57	0/13346

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	1620	1552	1545	8	0
1	B	1622	1567	1560	6	0
1	C	1615	1571	1564	8	0
1	D	1602	1568	1562	3	0
1	E	1575	1540	1534	11	0
1	F	1562	1512	1505	9	0
2	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	23	14	0	0	0
3	B	23	14	0	0	0
3	C	23	14	0	0	0
3	D	23	14	0	0	0
3	E	23	14	0	0	0
3	F	23	14	0	0	0
4	A	3	0	0	0	0
4	B	2	0	0	1	0
4	C	1	0	0	0	0
4	D	2	0	0	1	0
4	E	2	0	0	0	0
4	F	3	0	0	0	0
5	A	141	0	0	2	0
5	B	125	0	0	3	0
5	C	96	0	0	2	0
5	D	102	0	0	1	0
5	E	70	0	0	2	0
5	F	91	0	0	1	0
All	All	10378	9394	9270	47	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 2.

All (47) 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)
4:B:604:CL:CL	5:B:806:HOH:O	2.41	0.76
1:C:380:TYR:OH	5:C:701:HOH:O	2.09	0.70
1:B:380:TYR:OH	5:B:701:HOH:O	1.97	0.69
4:D:603:CL:CL	5:D:790:HOH:O	2.47	0.68
1:C:221:GLN:CG	1:C:268:THR:HG21	2.26	0.65
1:E:326[B]:CYS:SG	1:E:363:LEU:HD11	2.38	0.63
5:C:701:HOH:O	1:D:355:ASP:OD2	2.15	0.61
1:A:188:LEU:HD22	1:A:192:LYS:HD3	1.83	0.61
1:B:326[B]:CYS:SG	1:B:363:LEU:HD11	2.42	0.59
1:B:397:ALA:O	1:B:401:VAL:HG23	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:GLN:HG3	1:C:268:THR:HG21	1.85	0.58
1:C:326[B]:CYS:SG	1:C:363:LEU:HD11	2.42	0.58
1:E:398:ARG:O	1:E:401:VAL:HG12	2.03	0.57
1:C:221:GLN:HG2	1:C:268:THR:HG21	1.85	0.57
1:A:380:TYR:OH	5:A:701:HOH:O	2.00	0.57
1:C:278:ASP:OD1	1:C:281:ARG:NH1	2.38	0.56
1:A:278:ASP:OD1	1:A:281:ARG:NH2	2.38	0.54
1:A:326[B]:CYS:SG	1:A:363:LEU:HD11	2.50	0.51
1:A:235:PHE:O	1:A:236:THR:HG22	2.10	0.51
1:F:377:GLN:HG3	5:F:788:HOH:O	2.10	0.51
1:E:347:PRO:HB2	1:E:350:LYS:HG3	1.94	0.49
1:F:397:ALA:O	1:F:401:VAL:HG23	2.12	0.49
1:D:326[B]:CYS:SG	1:D:363:LEU:HD11	2.53	0.49
1:E:370[A]:ARG:HG2	5:E:762:HOH:O	2.13	0.48
1:A:188:LEU:HD22	1:A:192:LYS:CD	2.45	0.46
1:B:347:PRO:HB2	1:B:350:LYS:HG3	1.98	0.46
1:E:207:ILE:HD11	1:E:347:PRO:HG3	1.98	0.45
1:E:231:ASP:O	1:E:232:THR:OG1	2.31	0.45
5:A:829:HOH:O	1:F:311[B]:VAL:HG13	2.16	0.44
1:C:376:VAL:HG11	1:C:383:ARG:HH21	1.83	0.44
1:E:298:ALA:HA	1:E:388:VAL:HG12	1.99	0.44
1:F:298:ALA:HA	1:F:388:VAL:HG12	1.99	0.43
1:E:370[A]:ARG:HG3	5:E:754:HOH:O	2.18	0.42
1:E:292:ILE:HD13	1:E:323:CYS:SG	2.59	0.42
1:F:322:ARG:HD2	1:F:389:TRP:CG	2.55	0.42
1:A:347:PRO:HB2	1:A:350:LYS:HG3	2.02	0.42
1:F:292:ILE:HA	1:F:391:PHE:O	2.20	0.41
1:F:326[B]:CYS:SG	1:F:363:LEU:HD11	2.60	0.41
1:C:279:LEU:HD23	1:C:365:PHE:HZ	1.85	0.41
1:E:322:ARG:HD2	1:E:389:TRP:CG	2.55	0.41
1:F:258:TRP:CZ3	1:F:299:MET:HB2	2.56	0.41
1:A:326[A]:CYS:SG	1:A:365:PHE:CD2	3.12	0.41
1:B:376:VAL:HG11	1:B:383:ARG:NH2	2.36	0.41
1:E:223:GLY:HA2	1:E:330:LEU:CD1	2.51	0.41
1:F:260:GLU:HG2	1:F:297:LYS:HD3	2.03	0.40
1:D:322:ARG:HD2	1:D:389:TRP:CG	2.57	0.40
1:B:331:ASN:ND2	5:B:702:HOH:O	2.36	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	204/227 (90%)	197 (97%)	7 (3%)	0	100	100
1	B	205/227 (90%)	201 (98%)	4 (2%)	0	100	100
1	C	202/227 (89%)	198 (98%)	4 (2%)	0	100	100
1	D	201/227 (88%)	195 (97%)	6 (3%)	0	100	100
1	E	197/227 (87%)	194 (98%)	3 (2%)	0	100	100
1	F	196/227 (86%)	194 (99%)	2 (1%)	0	100	100
All	All	1205/1362 (88%)	1179 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	164/190 (86%)	161 (98%)	3 (2%)	59	48
1	B	167/190 (88%)	166 (99%)	1 (1%)	86	84
1	C	168/190 (88%)	168 (100%)	0	100	100
1	D	167/190 (88%)	165 (99%)	2 (1%)	71	65
1	E	164/190 (86%)	160 (98%)	4 (2%)	49	36
1	F	160/190 (84%)	158 (99%)	2 (1%)	69	62
All	All	990/1140 (87%)	978 (99%)	12 (1%)	73	65

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	THR
1	A	330	LEU
1	A	407	GLU
1	B	330	LEU
1	D	330	LEU
1	D	398	ARG
1	E	227[A]	ARG
1	E	227[B]	ARG
1	E	260	GLU
1	E	330	LEU
1	F	330	LEU
1	F	396	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 19 are monoatomic - leaving 6 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

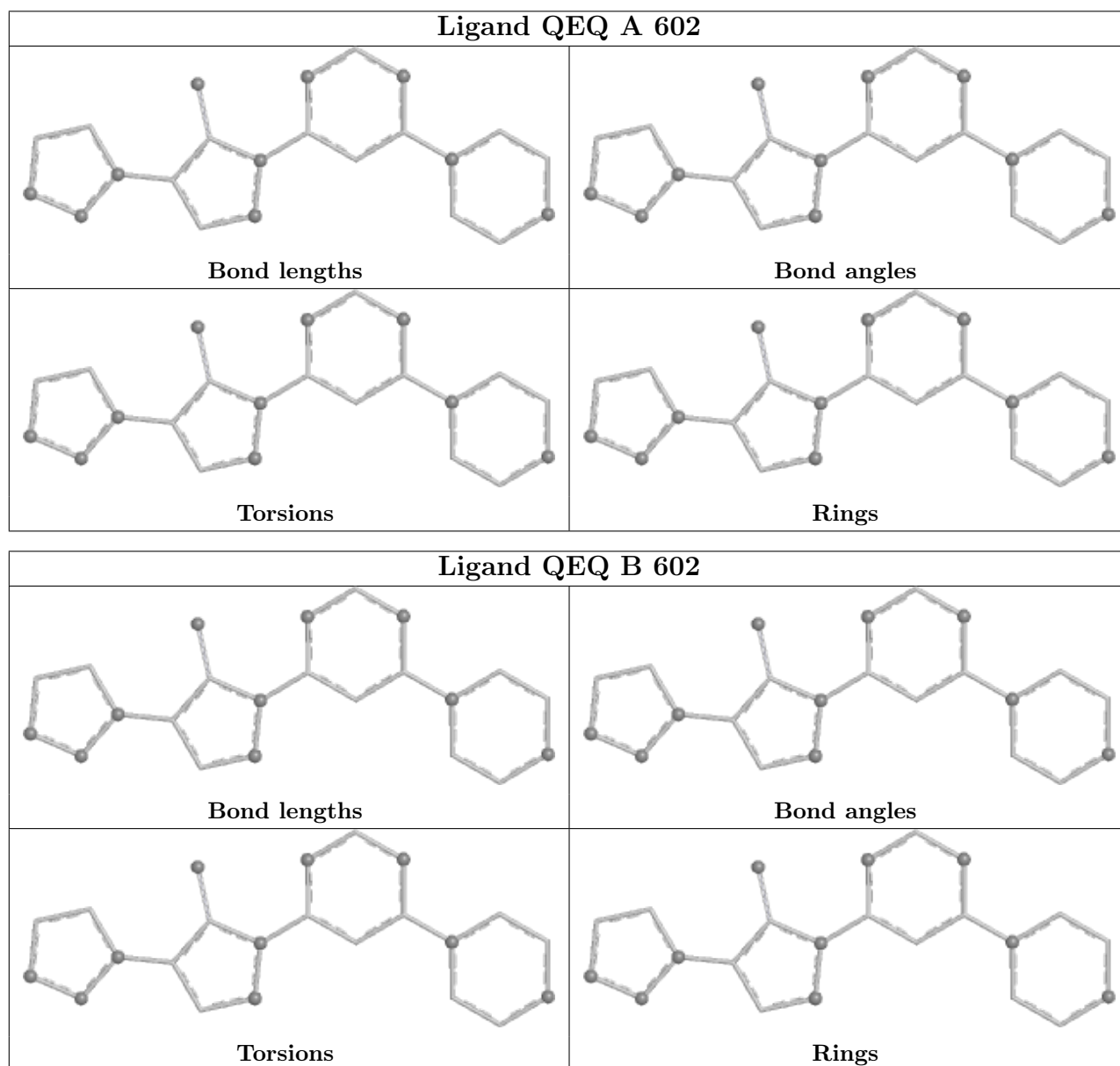
There are no chirality outliers.

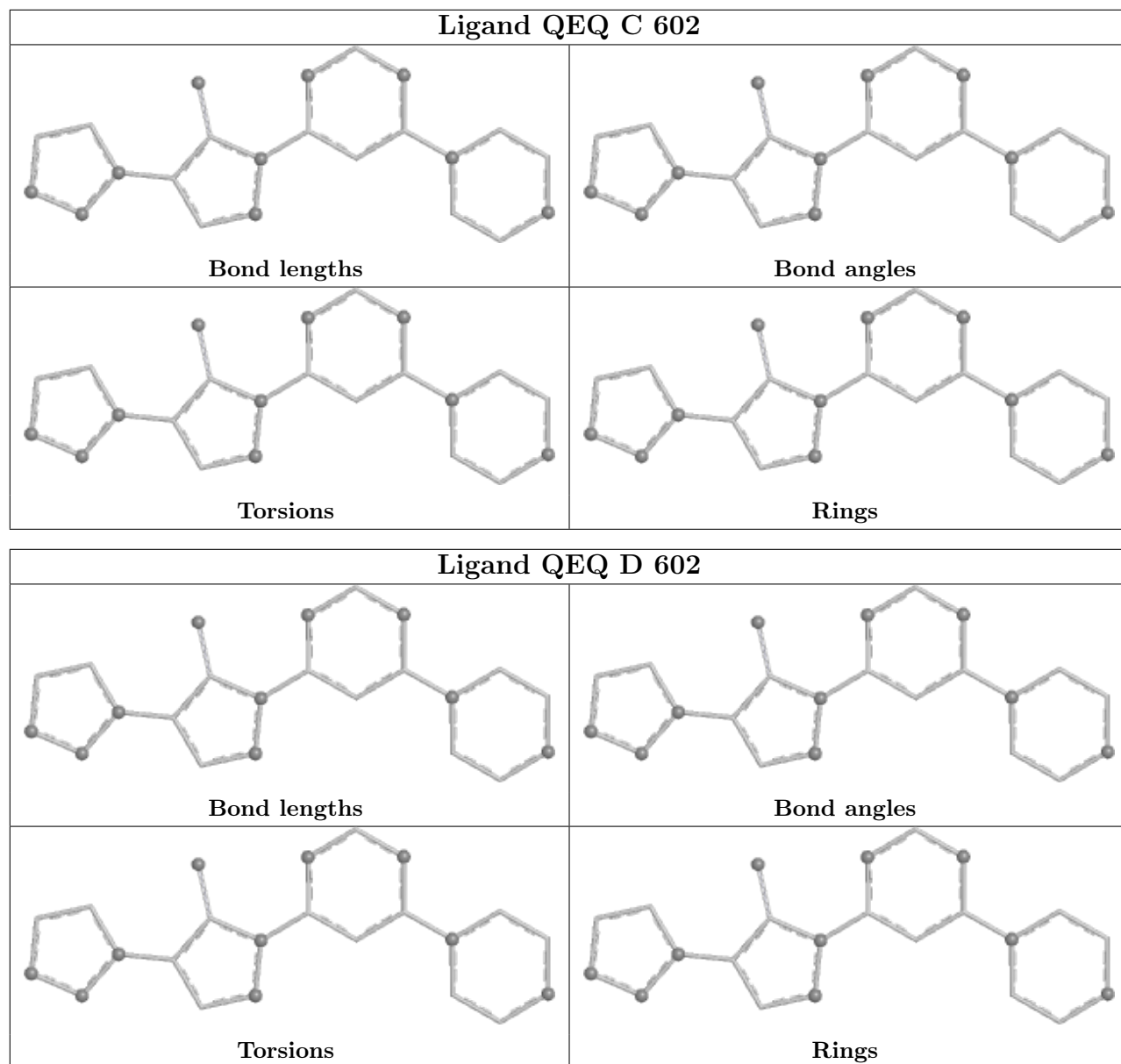
There are no torsion outliers.

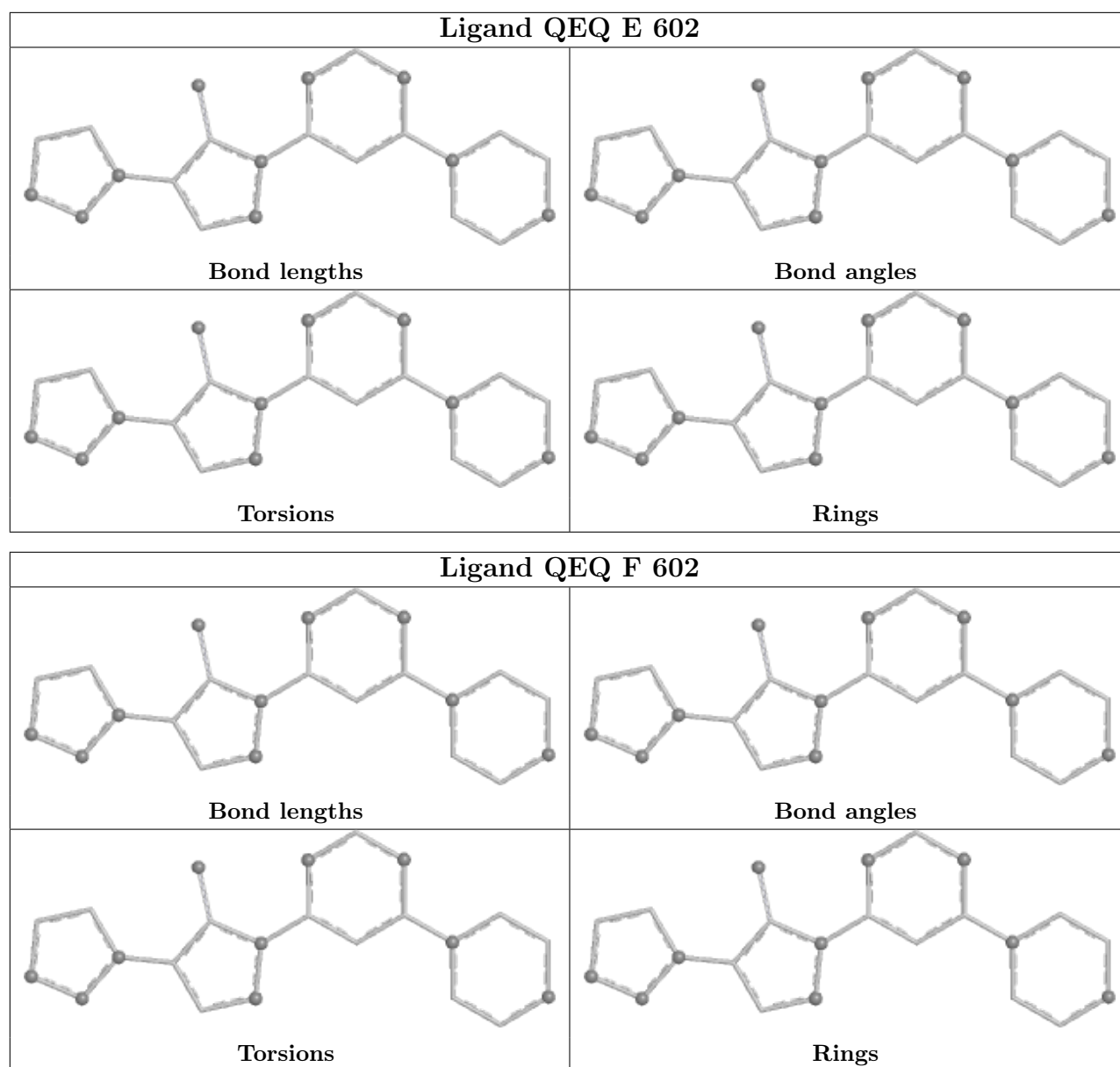
There are no ring outliers.

No monomer is involved in short contacts.

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	204/227 (89%)	0.71	11 (5%) 25 20	29, 43, 77, 120	0
1	B	205/227 (90%)	0.57	10 (4%) 29 24	32, 44, 69, 97	0
1	C	202/227 (88%)	0.55	11 (5%) 25 20	34, 52, 72, 94	0
1	D	202/227 (88%)	0.67	13 (6%) 19 15	35, 52, 78, 105	0
1	E	197/227 (86%)	0.86	22 (11%) 5 4	41, 61, 83, 103	0
1	F	196/227 (86%)	0.85	28 (14%) 2 1	33, 57, 84, 111	0
All	All	1206/1362 (88%)	0.70	95 (7%) 12 9	29, 51, 81, 120	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	188	LEU	10.1
1	A	236	THR	8.8
1	D	233	GLY	8.2
1	E	405	THR	6.5
1	A	233	GLY	5.9
1	E	189	PRO	5.5
1	E	404	LEU	5.2
1	A	235	PHE	4.8
1	D	232	THR	4.6
1	C	189	PRO	4.3
1	A	253	GLY	4.1
1	A	232	THR	4.0
1	B	232	THR	4.0
1	E	191	LEU	3.8
1	F	231	ASP	3.6
1	C	253	GLY	3.5
1	F	195	LEU	3.5
1	A	189	PRO	3.4
1	D	360	PHE	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	197	TYR	3.2
1	F	197	TYR	3.2
1	F	191	LEU	3.2
1	F	221	GLN	3.1
1	A	407	GLU	3.1
1	E	232	THR	3.1
1	C	192	LYS	3.1
1	B	188	LEU	3.1
1	A	234	LYS	3.0
1	F	229	LEU	3.0
1	C	191	LEU	3.0
1	E	401	VAL	3.0
1	F	189	PRO	2.9
1	D	235	PHE	2.9
1	C	284	ASN	2.9
1	F	227[A]	ARG	2.8
1	F	281	ARG	2.8
1	F	218	THR	2.8
1	E	271	LEU	2.8
1	D	188	LEU	2.8
1	F	217	GLU	2.8
1	C	330	LEU	2.7
1	D	236	THR	2.7
1	E	193	LEU	2.7
1	F	391	PHE	2.7
1	E	253	GLY	2.6
1	B	195	LEU	2.6
1	E	293	ASN	2.6
1	F	226	VAL	2.6
1	E	214	LEU	2.6
1	E	229	LEU	2.6
1	F	196	GLU	2.5
1	F	279	LEU	2.5
1	D	405	THR	2.4
1	F	220	GLN	2.4
1	E	388	VAL	2.4
1	C	195	LEU	2.4
1	F	405	THR	2.4
1	D	262	LYS	2.4
1	F	262	LYS	2.4
1	D	190	ALA	2.4
1	D	346	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	261	GLY	2.3
1	F	216	LYS	2.3
1	D	193	LEU	2.3
1	E	283	CYS	2.3
1	F	213	PHE	2.3
1	B	346	PHE	2.3
1	B	353	PHE	2.3
1	D	191	LEU	2.3
1	A	284	ASN	2.3
1	E	220	GLN	2.2
1	C	405	THR	2.2
1	F	222	ILE	2.2
1	C	237	ASP	2.2
1	B	407	GLU	2.2
1	F	267	GLU	2.2
1	B	404	LEU	2.2
1	F	271	LEU	2.2
1	E	272	LEU	2.1
1	E	195	LEU	2.1
1	E	192	LYS	2.1
1	C	222	ILE	2.1
1	C	376	VAL	2.1
1	E	380	TYR	2.1
1	B	184	GLN	2.1
1	F	272	LEU	2.1
1	D	192	LYS	2.0
1	E	190	ALA	2.0
1	E	275	SER	2.0
1	B	406	GLY	2.0
1	F	219	GLY	2.0
1	F	193	LEU	2.0
1	B	185	THR	2.0
1	F	258	TRP	2.0
1	A	406	GLY	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](#)

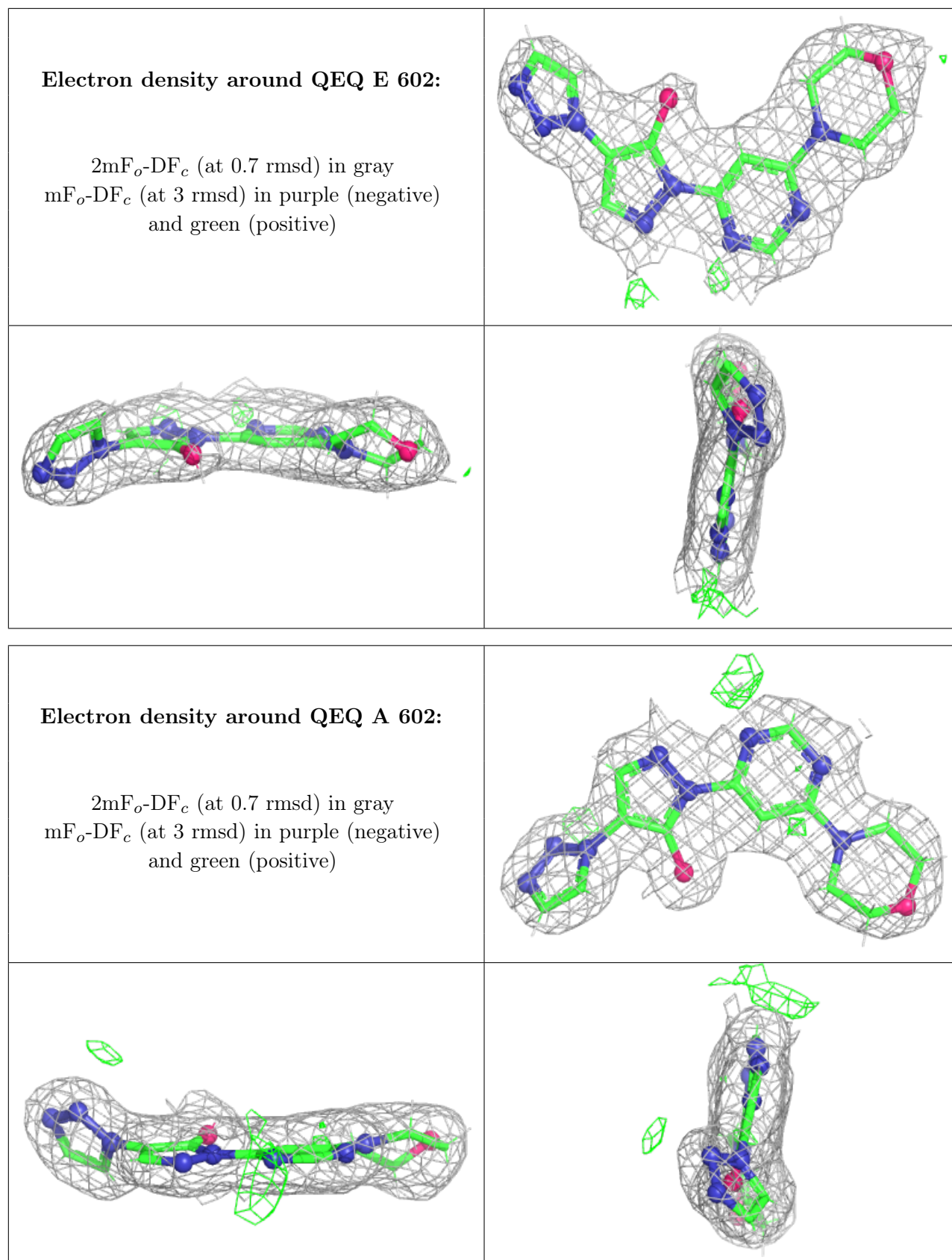
There are no monosaccharides in this entry.

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.

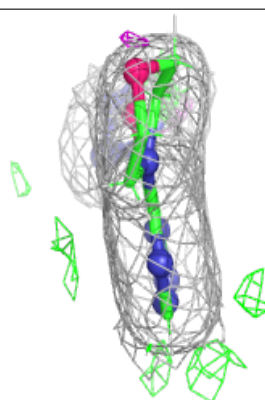
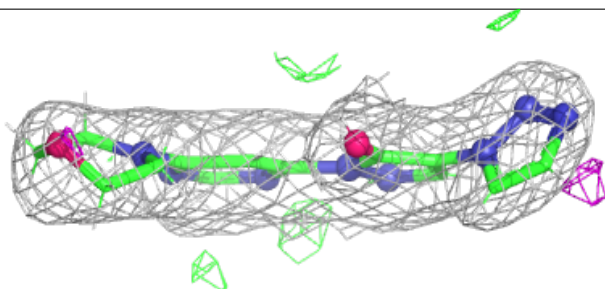
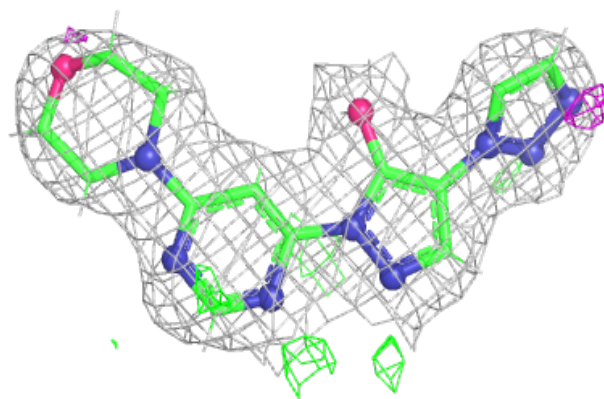
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CL	D	603	1/1	0.61	0.16	69,69,69,69	0
4	CL	F	604	1/1	0.66	0.10	70,70,70,70	0
4	CL	E	604	1/1	0.68	0.10	69,69,69,69	0
4	CL	A	605	1/1	0.81	0.05	70,70,70,70	0
4	CL	A	604	1/1	0.82	0.07	70,70,70,70	0
4	CL	B	604	1/1	0.83	0.08	67,67,67,67	0
4	CL	C	603	1/1	0.88	0.22	70,70,70,70	0
4	CL	B	603	1/1	0.90	0.12	50,50,50,50	0
4	CL	D	604	1/1	0.90	0.06	77,77,77,77	0
4	CL	E	603	1/1	0.92	0.13	58,58,58,58	0
4	CL	F	603	1/1	0.93	0.20	51,51,51,51	0
3	QEQ	E	602	23/23	0.94	0.12	41,50,63,65	0
4	CL	F	605	1/1	0.94	0.04	76,76,76,76	0
3	QEQ	A	602	23/23	0.95	0.12	32,38,54,57	0
3	QEQ	F	602	23/23	0.95	0.14	38,46,64,66	0
4	CL	A	603	1/1	0.95	0.15	50,50,50,50	0
3	QEQ	D	602	23/23	0.96	0.10	33,44,54,57	0
3	QEQ	B	602	23/23	0.97	0.10	28,38,51,52	0
3	QEQ	C	602	23/23	0.97	0.13	34,41,55,56	0
2	MN	E	601	1/1	0.98	0.18	39,39,39,39	0
2	MN	D	601	1/1	0.99	0.17	33,33,33,33	0
2	MN	B	601	1/1	0.99	0.19	30,30,30,30	0
2	MN	C	601	1/1	0.99	0.19	33,33,33,33	0
2	MN	F	601	1/1	1.00	0.20	35,35,35,35	0
2	MN	A	601	1/1	1.00	0.18	28,28,28,28	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.

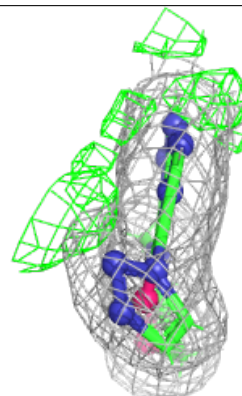
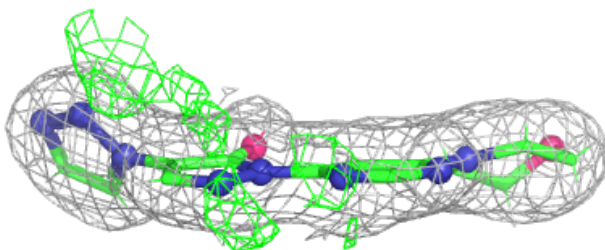
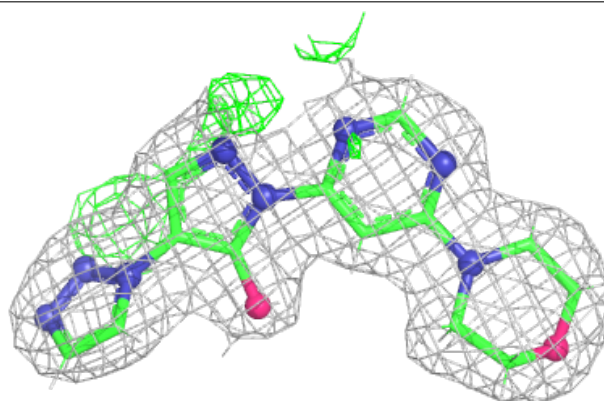


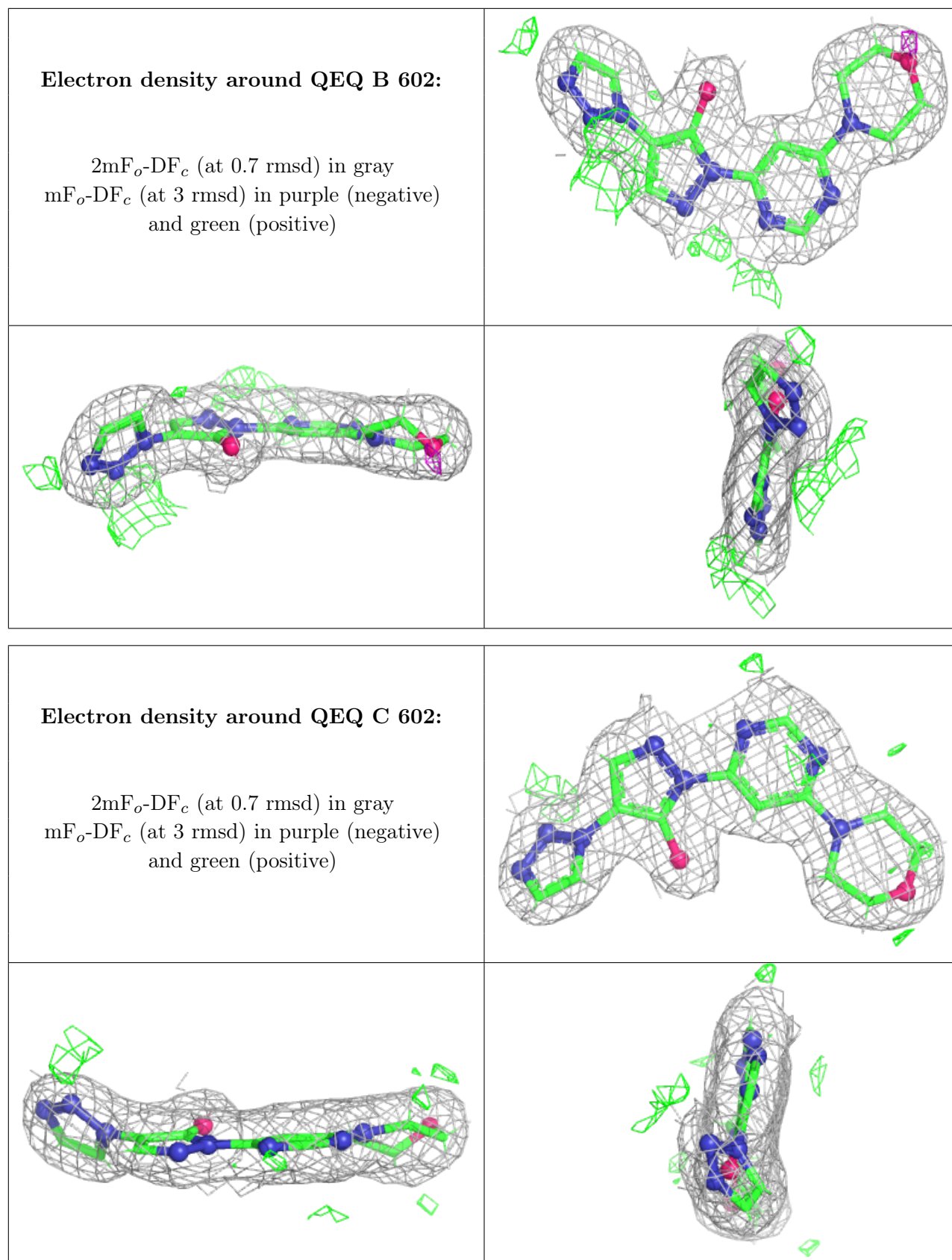
Electron density around QEQ F 602:

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

**Electron density around QEQ D 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.