



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:54 PM UTC

PDB ID : 6ULA / pdb_00006ula
Title : Crystal structure of human GAC in complex with inhibitor UPGL00012
Authors : Huang, Q.; Cerione, R.A.
Deposited on : 2019-10-07
Resolution : 2.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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

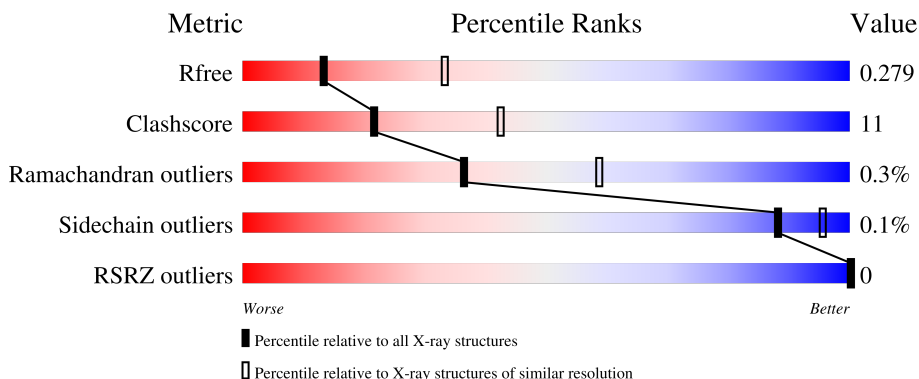
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	527	 59% 18% 22%
1	B	527	 60% 17% 22%
1	C	527	 60% 16% 22%
1	D	527	 59% 18% 22%
1	E	527	 62% 15% 22%

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Mol	Chain	Length	Quality of chain			
1	F	527		61%	17%	22%
1	G	527		60%	17%	22%
1	H	527		62%	16%	22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	QA4	A	601	-	X	-	-
2	QA4	E	601	-	X	-	-

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 25668 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.

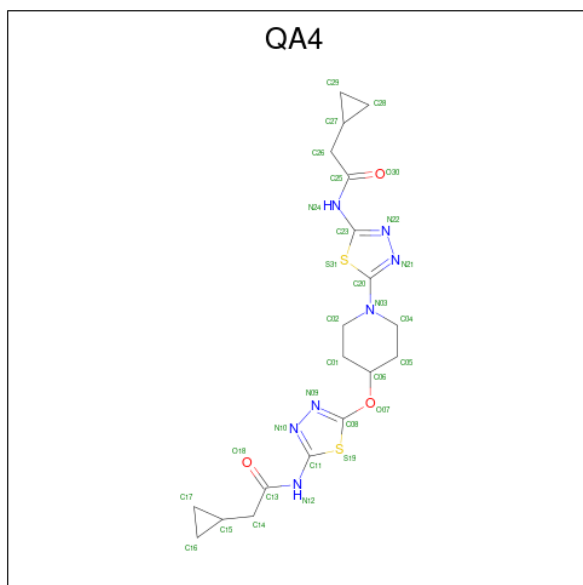
- Molecule 1 is a protein called Glutaminase kidney isoform, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	409	3190	2034	539	589	28	1	0	0
1	B	410	3194	2036	540	590	28	1	0	0
1	C	410	3194	2036	540	590	28	1	0	0
1	D	410	3194	2036	540	590	28	1	0	0
1	E	409	3190	2034	539	589	28	1	0	0
1	G	410	3194	2036	540	590	28	1	0	0
1	F	410	3194	2036	540	590	28	1	0	0
1	H	410	3194	2036	540	590	28	1	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	268	ALA	VAL	conflict	UNP O94925
B	268	ALA	VAL	conflict	UNP O94925
C	268	ALA	VAL	conflict	UNP O94925
D	268	ALA	VAL	conflict	UNP O94925
E	268	ALA	VAL	conflict	UNP O94925
G	268	ALA	VAL	conflict	UNP O94925
F	268	ALA	VAL	conflict	UNP O94925
H	268	ALA	VAL	conflict	UNP O94925

- Molecule 2 is 2-cyclopropyl-N-{5-[4-({5-[(cyclopropylacetyl)amino]-1,3,4-thiadiazol-2-yl}oxy)piperidin-1-yl]-1,3,4-thiadiazol-2-yl}acetamide (CCD ID: QA4) (formula: C₁₉H₂₅N₇O₃S₂) (labeled as "Ligand of Interest" by depositor).

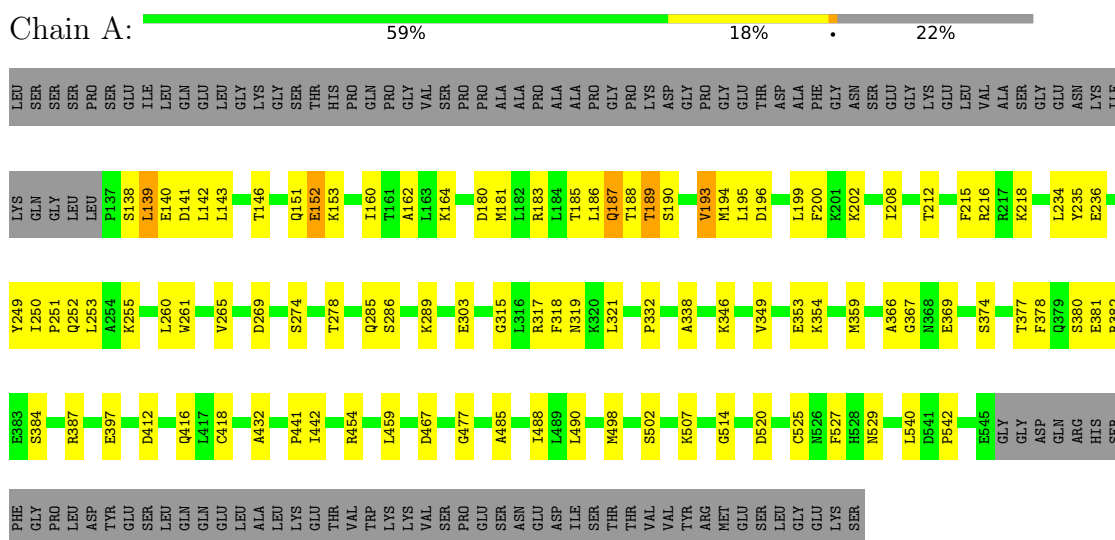


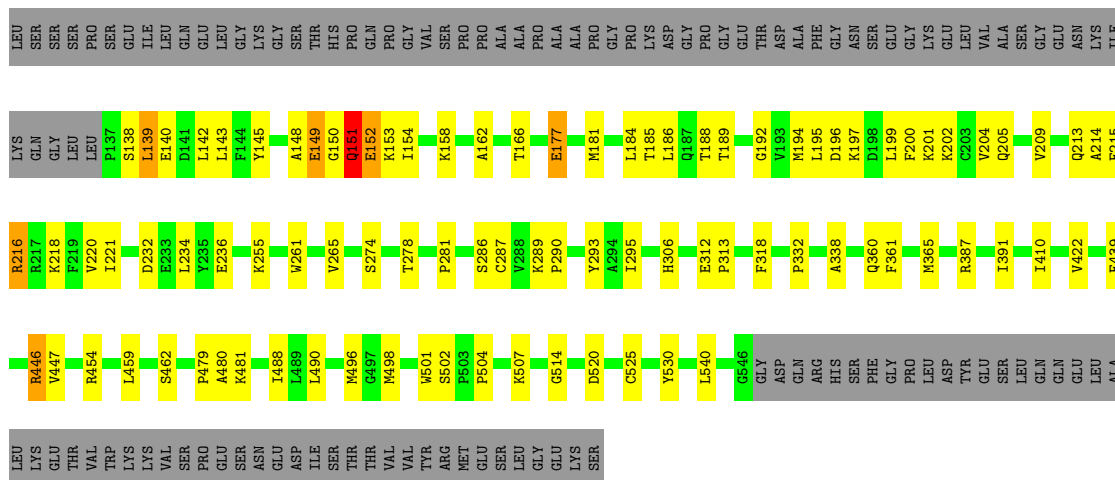
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			31	19	7	3	2		
2	C	1	Total	C	N	O	S	0	0
			31	19	7	3	2		
2	E	1	Total	C	N	O	S	0	0
			31	19	7	3	2		
2	E	1	Total	C	N	O	S	0	0
			31	19	7	3	2		

3 Residue-property plots [i](#)

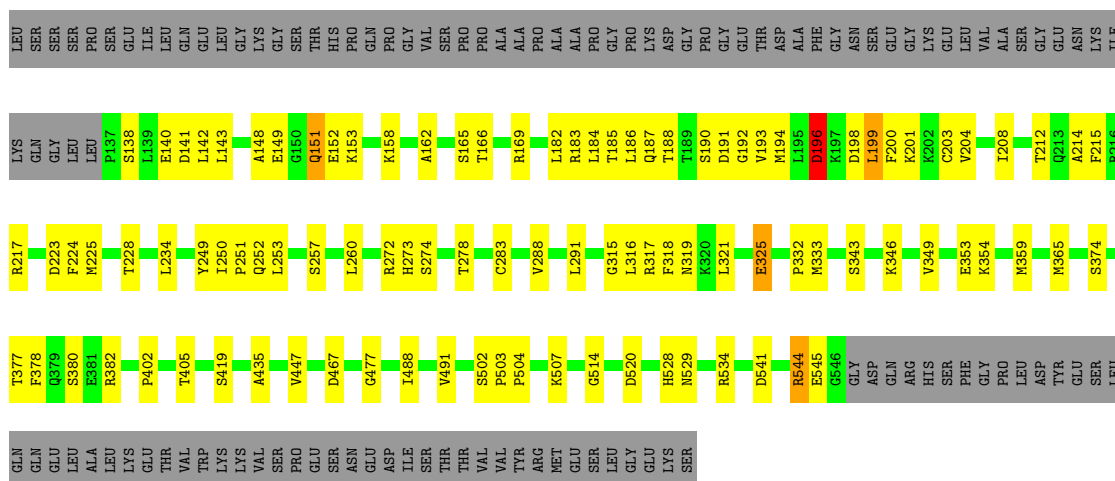
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

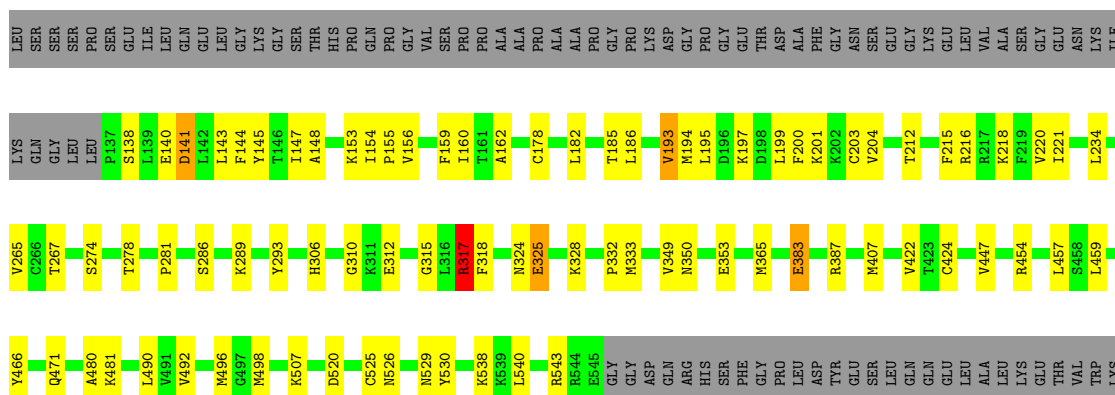




• Molecule 1: Glutaminase kidney isoform, mitochondrial



• Molecule 1: Glutaminase kidney isoform, mitochondrial



LYS
VAL
SER
SER
PRO
GLU
SER
SER
ASN
GLU
ASP
ILE
SER
SER
THR
THR
VAL
VAL
TYR
ARG
MET
MET
GLU
SER
SER
GLY
GLY
LYS
SER

- Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain G: 60% 17% 22%

LEU
SER
SER
SER
LEU
PRO
SER
SER
ILE
LEU
GLN
GLU
GLU
LEU
GLY
LYS
GLY
SER
SER
THR
HIS
HIS
PRO
GLN
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SER
PRO
PRO
ALA
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ALA
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LYS
ASP
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PHE
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SER
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GLY
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VAL
VAL
ALA
SER
SER
GLY
GLU
ASN
LYS
ILE

LYS
GLN
GLY
LEU
LEU
LEU
P137
S138
L139
L140
D141
L142
L143
F144
I147
E152
K153
I154
P155
V156
H157
K158
A162
T166
R169
L175
M181
L184
T185
T188
T189
S190
D191
G192
V193
M194
L195
K201
K202
A214
F215
F224
F227
T228
L234
A247

V248
Y249
I250
V265
R272
H273
S274
T278
T278
C283
L284
Q285
S286
C287
V288
K289
P289
L291
Y304
Y306
R307
K311
G315
L316
R317
F318
N319
P332
M333
V340
V341
T342
S343
L344
V349
N350
E353
L362
M365
A366
E369
S374
T377
F378

G379
S380
S384
E397
K398
P402
Q416
S419
V447
D467
G477
V484
L488
M496
G497
M498
G514
F517
D520
H528
N529
A537
R544
E545
G546
GLY
ASN
GLN
ARG
HIS
SER
PHE
GLY
PRO
LEU
VAL
ASP
TYR
GLU
LEU
GLN
GLY

LEU
ALA
LEU
LYS
THR
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TRP
LYS
VAL
SER
PRO
GLU
GLY
SER
ASN
THR
ASP
PRO
ILE
SER
THR
VAL
VAL
VAL
TYR
ARG
MET
GLU
SER
LEU
GLY
GLY
LYS
SER

- Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain F: 61% 17% 22%

LEU
SER
SER
SER
LEU
PRO
SER
SER
ILE
LEU
GLN
GLU
GLU
LEU
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PRO
VAL
GLY
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ALA
ALA
PRO
GLY
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ASP
GLY
PRO
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ASN
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GLU
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LYS
GLU
LEU
VAL
VAL
ALA
ALA
SER
SER
GLY
GLU
ASN
LYS
ILE

LYS
GLN
GLY
LEU
LEU
LEU
P137
E140
L143
F144
Y145
T146
I147
A148
E152
P155
H156
K158
F159
I160
T161
A162
T166
E177
M181
L182
R183
L184
T185
L186
Q187
T188
T189
S190
D191
G192
W193
M194
L195
L199
F200
K201
K202
C203
Q204
Q205
S206
N207
A214
R216

R217
K218
F224
T228
L234
K245
D248
Y249
I250
L253
K255
F256
S257
P258
V265
S274
T278
V280
Q285
S286
C287
K289
K289
K292
E303
E312
R317
F318
L321
A338
S343
V349
N350
E353
K354
F355
M365

E383
R387
E397
I410
I420
C424
E425
V447
P450
R454
Y466
D467
F468
Q471
F472
G477
I488
L489
L490
M498
G514
D520
M529
G546
ASP
GLN
ARG
SER
PHE
GLY
PRO
LEU
ASP
TYR
GLU
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LEU
GLN
GLY
GLY
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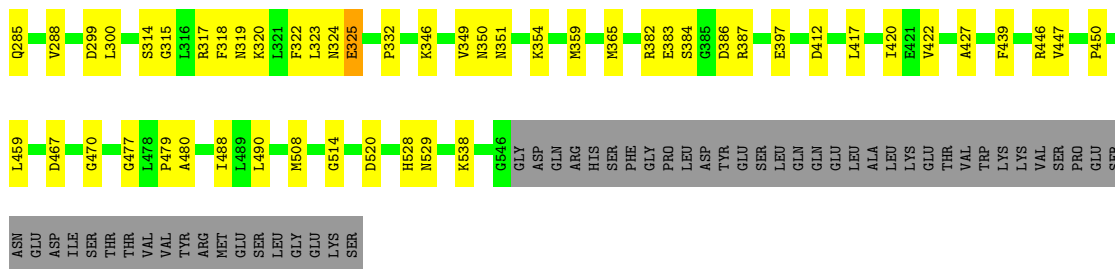
ALA
LEU
GLY
THR
VAL
TRP
LYS
VAL
SER
PRO
GLU
SER
ASN
GLU
ASP
ILE
THR
THR
VAL
VAL
TYR
ARG
MET
GLU
SER
LEU
GLY
GLY
LYS
SER

- Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain H: 62% 16% 22%

LEU
SER
SER
SER
PRO
SER
SER
ILE
LEU
GLN
GLU
GLU
LEU
GLY
LYS
GLY
SER
SER
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GLY
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SER
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THR
ASP
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LEU
VAL
ALA
SER
SER
GLY
GLU
ASN
LYS
ILE

LYS
GLN
GLY
LEU
LEU
LEU
P137
E140
L143
F144
Y145
A148
E149
G150
Q151
E152
K153
V156
H157
K158
A162
R174
L182
G192
M193
M194
L195
D196
K197
D198
L199
K202
C203
V208
L210
L211
T212
F215
R216
R217
L234
K255
S274
T278



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.72Å 138.89Å 177.15Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	37.89 – 2.95 37.89 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.1 (37.89-2.95) 97.4 (37.89-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.217 , 0.279 0.219 , 0.279	Depositor DCC
R_{free} test set	1992 reflections (1.57%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtrriage
Anisotropy	0.264	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 17.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.438 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	25668	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3974e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: QA4

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	0.47	0/3262	0.77	4/4403 (0.1%)
1	B	0.51	1/3266 (0.0%)	0.81	8/4408 (0.2%)
1	C	0.52	2/3266 (0.1%)	0.85	14/4408 (0.3%)
1	D	0.53	1/3266 (0.0%)	0.80	6/4408 (0.1%)
1	E	0.56	2/3262 (0.1%)	0.83	14/4403 (0.3%)
1	F	0.60	5/3266 (0.2%)	0.85	11/4408 (0.2%)
1	G	0.48	0/3266	0.86	11/4408 (0.2%)
1	H	0.52	0/3266	0.89	11/4408 (0.2%)
All	All	0.52	11/26120 (0.0%)	0.83	79/35254 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	3
1	F	0	1
All	All	0	8

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	317	ARG	CZ-NH2	11.96	1.49	1.33
1	F	255	LYS	CD-CE	10.46	1.83	1.52
1	F	280	VAL	CA-C	9.39	1.60	1.53
1	E	317	ARG	CZ-NH1	-7.65	1.22	1.32
1	F	280	VAL	C-N	-7.23	1.24	1.33

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	280	VAL	CA-C-O	-11.82	112.18	119.15
1	G	317	ARG	CA-CB-CG	-11.65	90.80	114.10
1	F	317	ARG	CB-CG-CD	-10.98	86.05	111.30
1	H	325	GLU	CA-CB-CG	10.55	135.19	114.10
1	H	151	GLN	CA-C-N	-10.07	106.88	122.49

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	317	ARG	Sidechain
1	C	151	GLN	Peptide
1	D	151	GLN	Peptide
1	D	190	SER	Peptide
1	E	317	ARG	Sidechain

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	3190	0	3167	82	0
1	B	3194	0	3170	68	0
1	C	3194	0	3170	71	0
1	D	3194	0	3170	82	0
1	E	3190	0	3165	66	0
1	F	3194	0	3170	72	0
1	G	3194	0	3170	71	0
1	H	3194	0	3170	79	0
2	A	31	0	0	1	0
2	C	31	0	0	0	0
2	E	62	0	0	2	0
All	All	25668	0	25352	553	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 11.

The worst 5 of 553 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:F:255:LYS:CE	1:F:255:LYS:CD	1.83	1.55
1:F:255:LYS:CE	1:F:255:LYS:NZ	1.68	1.51
1:F:250:ILE:HD11	1:F:253:LEU:HG	1.22	1.17
1:H:467:ASP:CB	1:H:508:MET:CE	2.27	1.12
1:H:467:ASP:HB3	1:H:508:MET:HE1	1.18	1.12

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	407/527 (77%)	393 (97%)	11 (3%)	3 (1%)	18	40
1	B	408/527 (77%)	392 (96%)	16 (4%)	0	100	100
1	C	408/527 (77%)	397 (97%)	10 (2%)	1 (0%)	43	66
1	D	408/527 (77%)	393 (96%)	13 (3%)	2 (0%)	24	49
1	E	407/527 (77%)	397 (98%)	9 (2%)	1 (0%)	43	66
1	F	408/527 (77%)	396 (97%)	11 (3%)	1 (0%)	43	66
1	G	408/527 (77%)	394 (97%)	13 (3%)	1 (0%)	43	66
1	H	408/527 (77%)	397 (97%)	10 (2%)	1 (0%)	43	66
All	All	3262/4216 (77%)	3159 (97%)	93 (3%)	10 (0%)	36	59

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	191	ASP
1	H	196	ASP
1	A	152	GLU
1	G	192	GLY

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Continued from previous page...

Mol	Chain	Res	Type
1	F	188	THR

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	353/451 (78%)	353 (100%)	0	100	100
1	B	353/451 (78%)	353 (100%)	0	100	100
1	C	353/451 (78%)	352 (100%)	1 (0%)	86	92
1	D	353/451 (78%)	353 (100%)	0	100	100
1	E	353/451 (78%)	352 (100%)	1 (0%)	86	92
1	F	353/451 (78%)	353 (100%)	0	100	100
1	G	353/451 (78%)	353 (100%)	0	100	100
1	H	353/451 (78%)	353 (100%)	0	100	100
All	All	2824/3608 (78%)	2822 (100%)	2 (0%)	88	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	177	GLU
1	E	147	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	516	HIS
1	F	516	HIS
1	F	471	GLN
1	H	319	ASN
1	C	351	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
2	QA4	C	601	-	35,35,35	2.24	13 (37%)	47,49,49	4.26	23 (48%)
2	QA4	E	601	-	35,35,35	2.95	15 (42%)	47,49,49	5.98	28 (59%)
2	QA4	E	602	-	35,35,35	2.10	17 (48%)	47,49,49	4.33	20 (42%)
2	QA4	A	601	-	35,35,35	2.23	14 (40%)	47,49,49	4.00	28 (59%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	QA4	C	601	-	-	8/22/38/38	0/5/5/5
2	QA4	E	601	-	-	14/22/38/38	0/5/5/5
2	QA4	E	602	-	-	8/22/38/38	0/5/5/5
2	QA4	A	601	-	-	9/22/38/38	0/5/5/5

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	QA4	C25-N24	10.26	1.56	1.37
2	E	601	QA4	C20-N03	5.48	1.46	1.34
2	A	601	QA4	C08-N09	5.38	1.35	1.29
2	E	601	QA4	O07-C08	5.27	1.42	1.35
2	E	601	QA4	C11-N12	5.07	1.45	1.38

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	QA4	N24-C23-N22	19.77	138.46	120.81
2	E	602	QA4	C06-O07-C08	-17.53	106.19	117.71
2	E	601	QA4	C25-N24-C23	13.55	146.85	123.69
2	C	601	QA4	N24-C23-N22	12.26	131.76	120.81
2	E	601	QA4	S31-C23-N22	-11.15	102.07	114.52

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	QA4	S19-C11-N12-C13
2	A	601	QA4	N12-C13-C14-C15
2	A	601	QA4	O18-C13-C14-C15
2	A	601	QA4	N24-C25-C26-C27
2	A	601	QA4	O30-C25-C26-C27

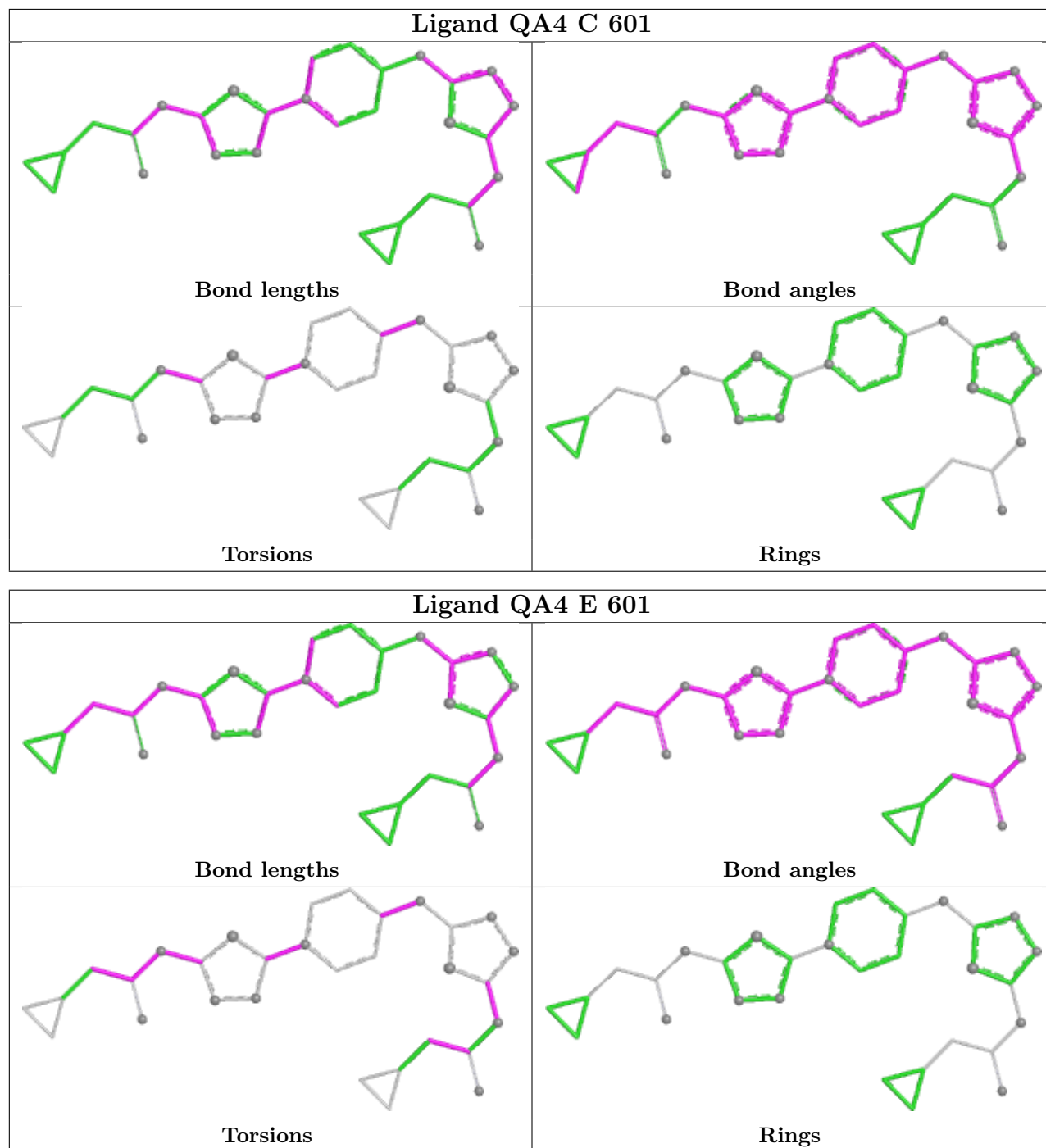
There are no ring outliers.

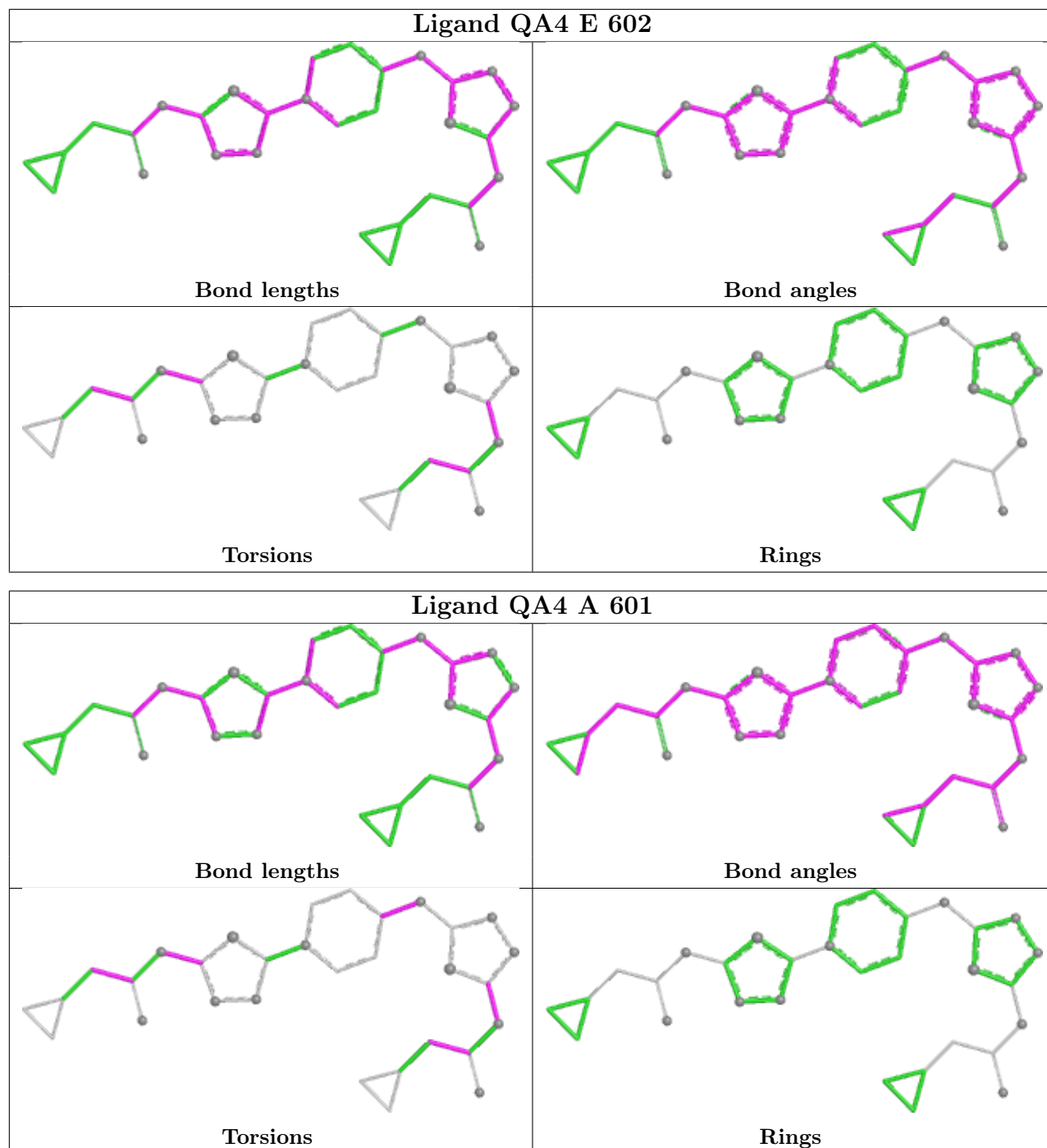
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	601	QA4	2	0
2	A	601	QA4	1	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	409/527 (77%)	-1.57	0 100 100	25, 42, 100, 171	0
1	B	410/527 (77%)	-1.59	0 100 100	27, 41, 91, 152	0
1	C	410/527 (77%)	-1.57	0 100 100	27, 42, 96, 167	0
1	D	410/527 (77%)	-1.56	0 100 100	27, 41, 95, 155	0
1	E	409/527 (77%)	-1.60	0 100 100	26, 41, 88, 171	0
1	F	410/527 (77%)	-1.55	0 100 100	28, 42, 101, 162	0
1	G	410/527 (77%)	-1.56	0 100 100	28, 43, 95, 165	0
1	H	410/527 (77%)	-1.58	0 100 100	25, 42, 97, 175	0
All	All	3278/4216 (77%)	-1.57	0 100 100	25, 42, 97, 175	0

There are no RSRZ outliers to report.

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](#)

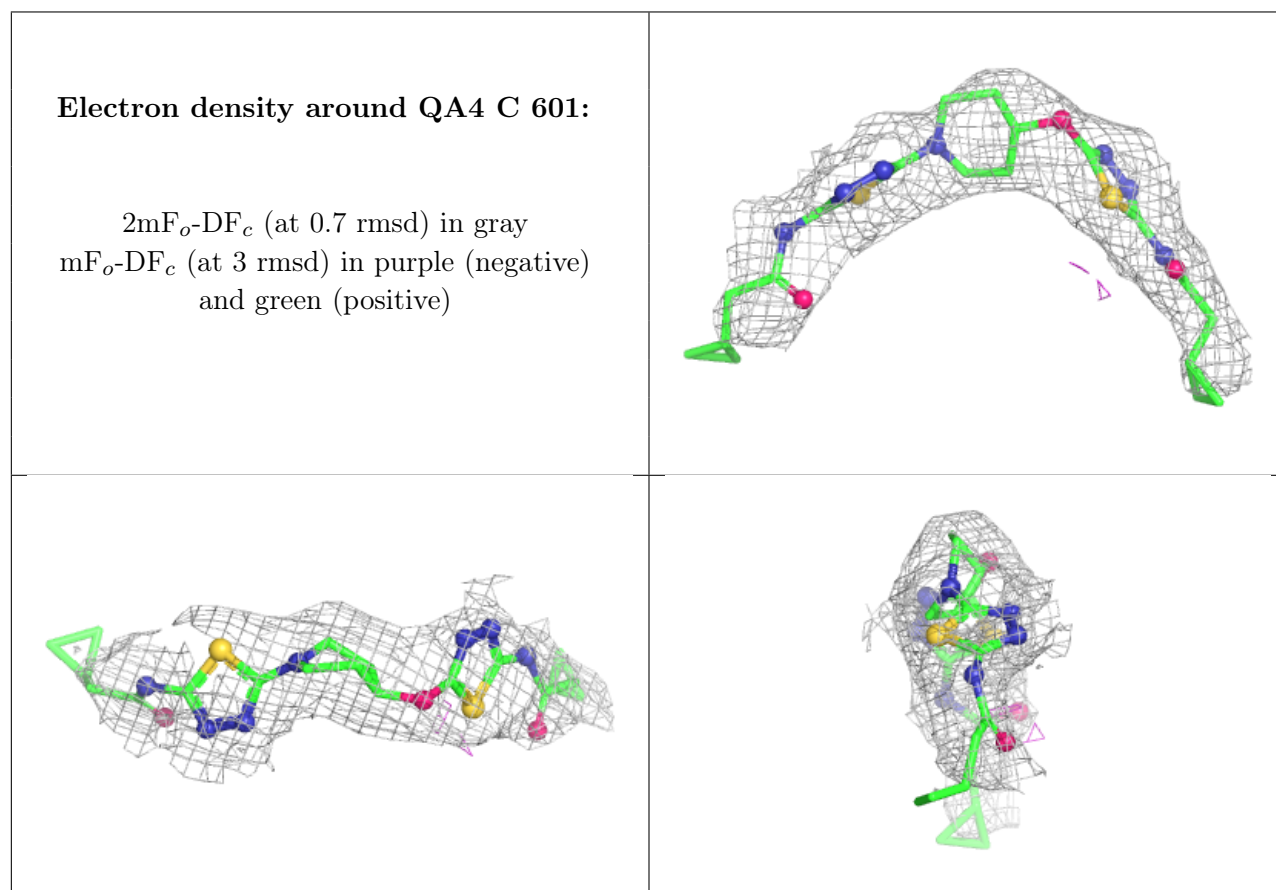
There are no oligosaccharides in this entry.

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.

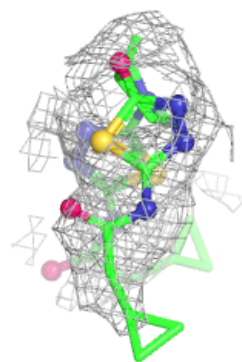
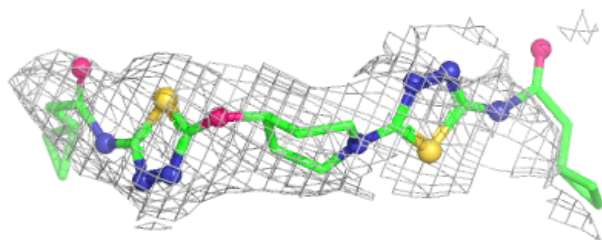
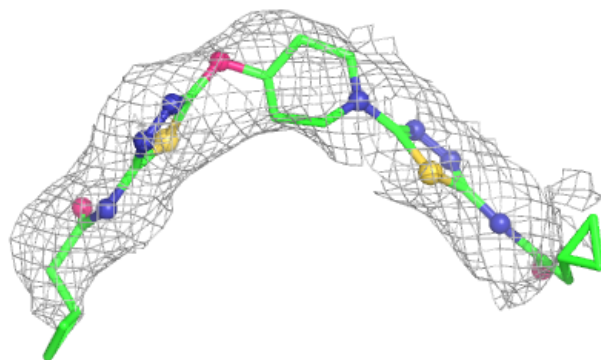
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	QA4	C	601	31/31	0.99	0.04	45,58,100,102	0
2	QA4	E	601	31/31	0.99	0.04	53,63,120,157	0
2	QA4	E	602	31/31	0.99	0.04	44,62,75,78	0
2	QA4	A	601	31/31	1.00	0.04	47,60,83,85	0

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.

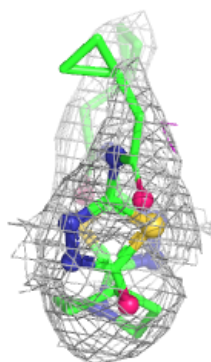
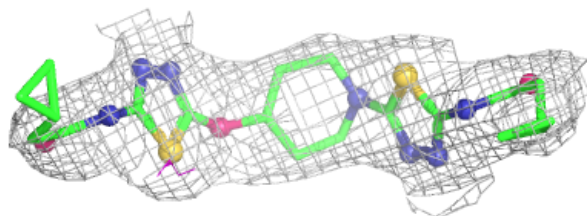
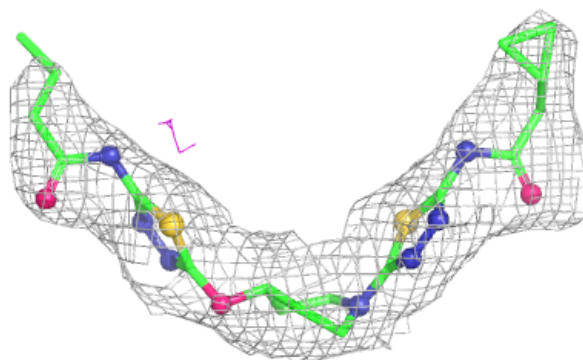


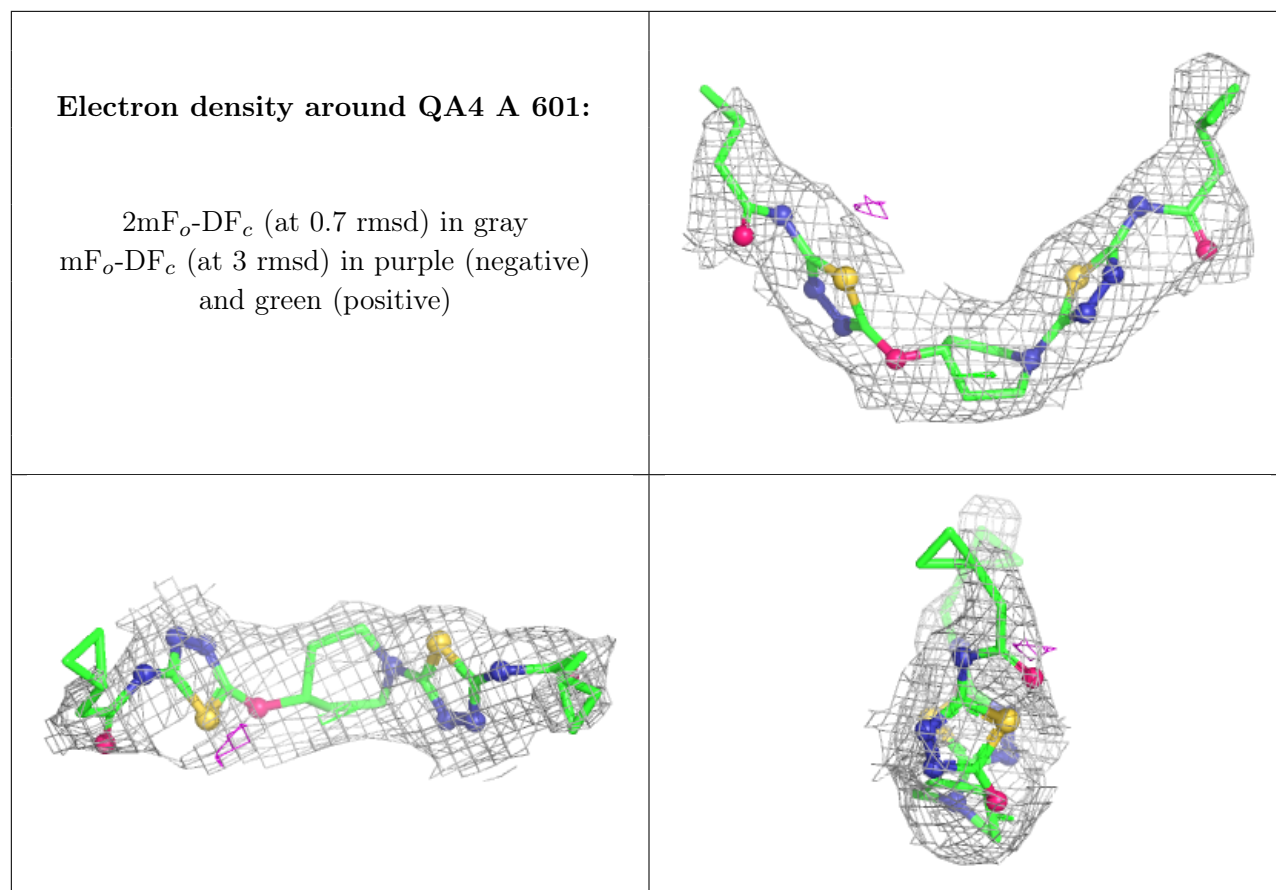
Electron density around QA4 E 601:

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

**Electron density around QA4 E 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.