wwPDB X-ray Structure Validation Summary Report (i)

Dec 16, 2024 – 06:59 AM EST

PDB ID	:	6ULA
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.

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 (i) 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 (i)) were used in the production of this report:

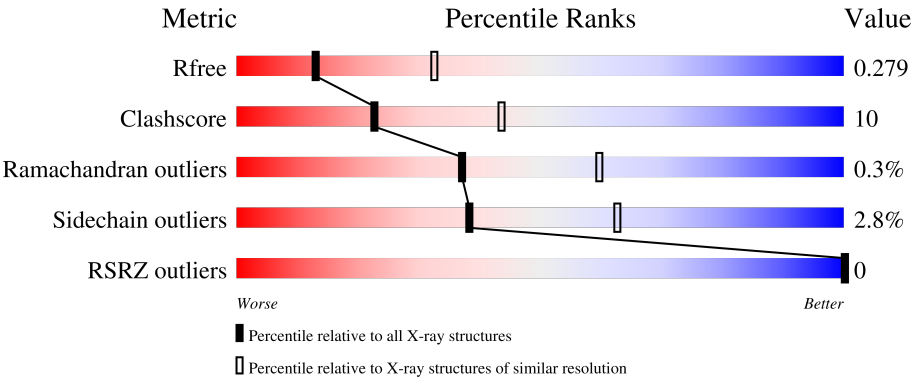
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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}	164625	1044 (2.98-2.94)
Clashscore	180529	1097 (2.98-2.94)
Ramachandran outliers	177936	1049 (2.98-2.94)
Sidechain outliers	177891	1049 (2.98-2.94)
RSRZ outliers	164620	1044 (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 <=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	58% 18% • 22%
1	B	527	60% 16% • 22%
1	C	527	61% 15% •• 22%
1	D	527	59% 16% •• 22%
1	E	527	62% 15% • 22%

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Mol	Chain	Length	Quality of chain
1	F	527	59% 17% 22%
1	G	527	60% 16% 22%
1	H	527	61% 15% 22%

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.

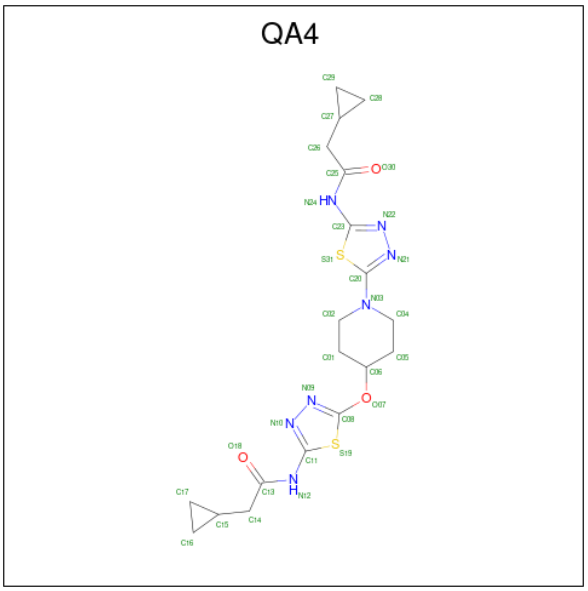
- Molecule 1 is a protein called Glutaminase kidney isoform, mitochondrial.

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

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 (three-letter code: QA4) (formula: $C_{19}H_{25}N_7O_3S_2$) (labeled as "Ligand of Interest" by depositor).



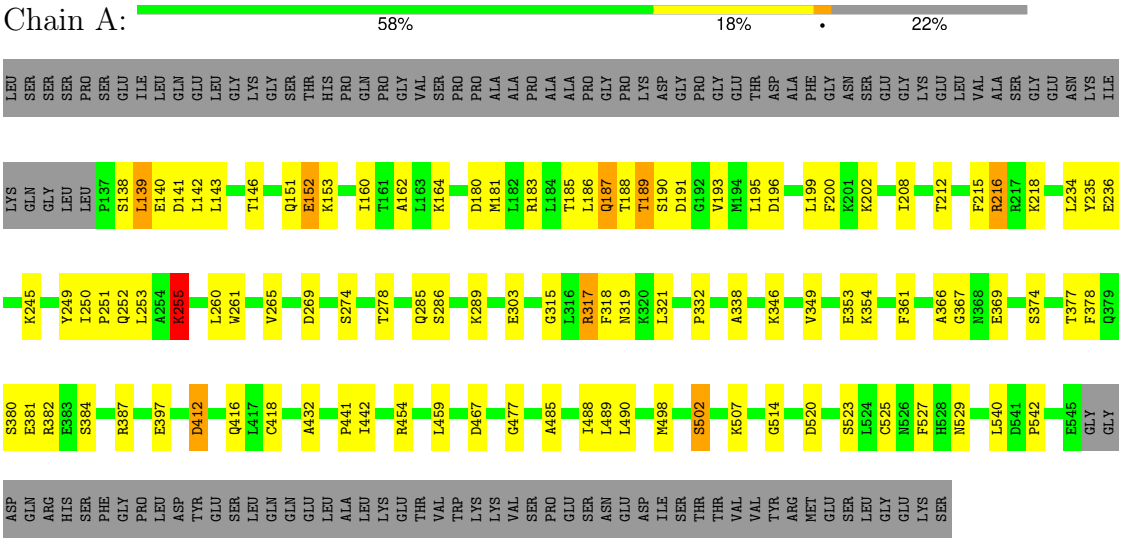
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			31	19	7	3	2		
2	C	1	Total	C	N	O	S	0	0
			31	19	7	3	2		
2	E	1	Total	C	N	O	S	0	0
			31	19	7	3	2		
2	E	1	Total	C	N	O	S	0	0
			31	19	7	3	2		

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.

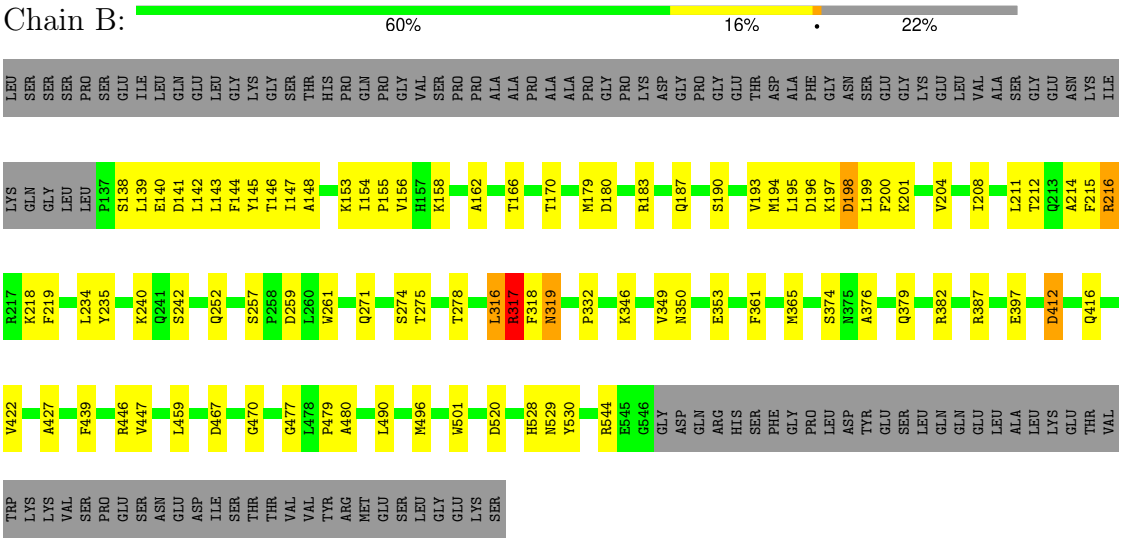
• Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain A:



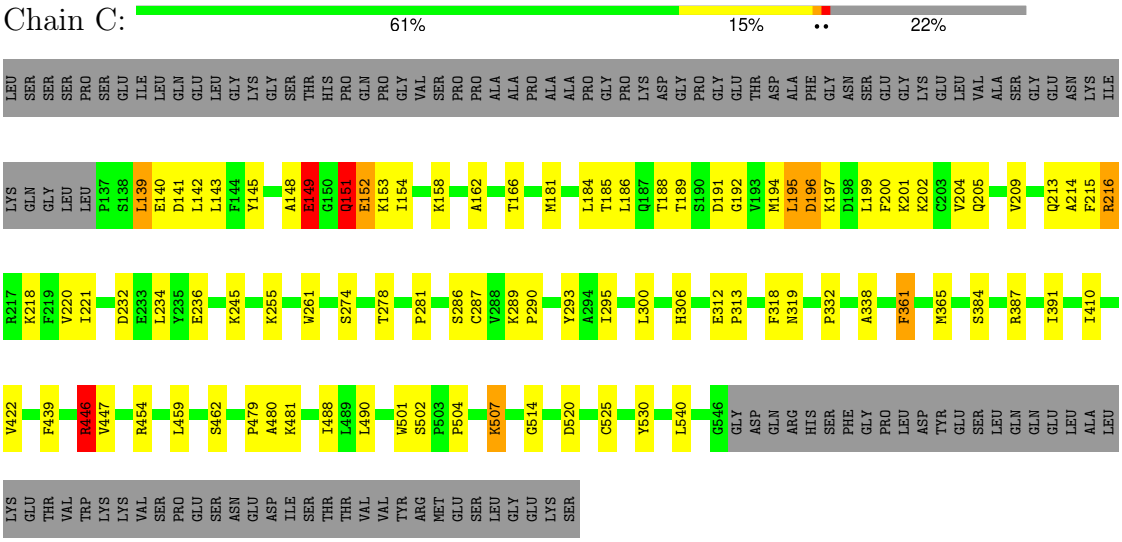
• Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain B:



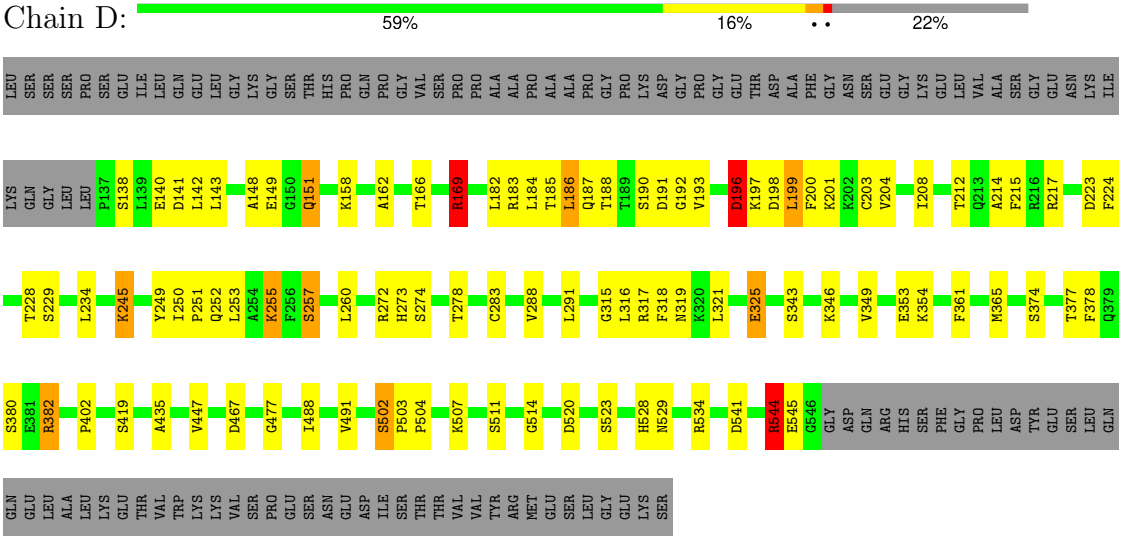
• Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain C:



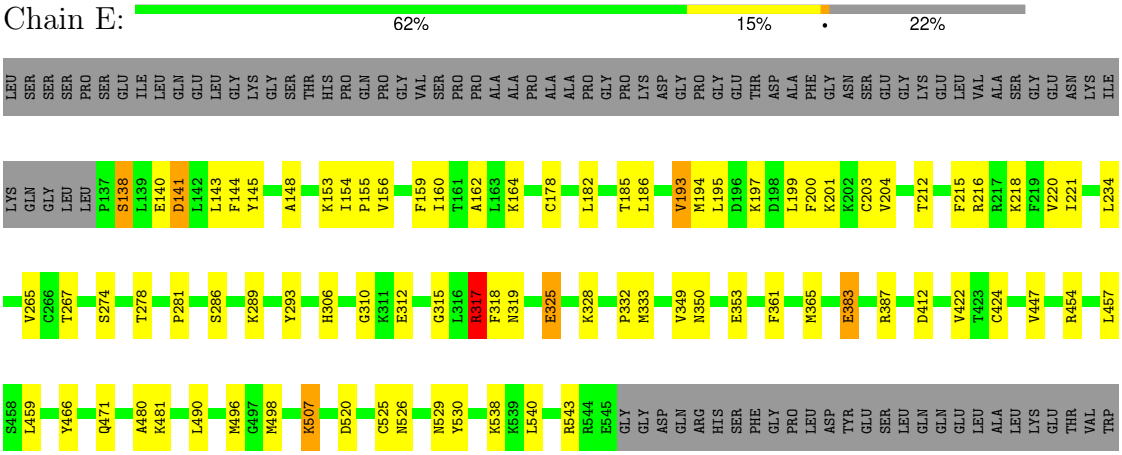
• Molecule 1: Glutaminase kidney isoform, mitochondrial

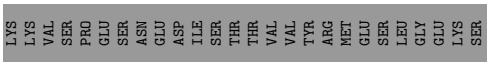
Chain D:



• Molecule 1: Glutaminase kidney isoform, mitochondrial

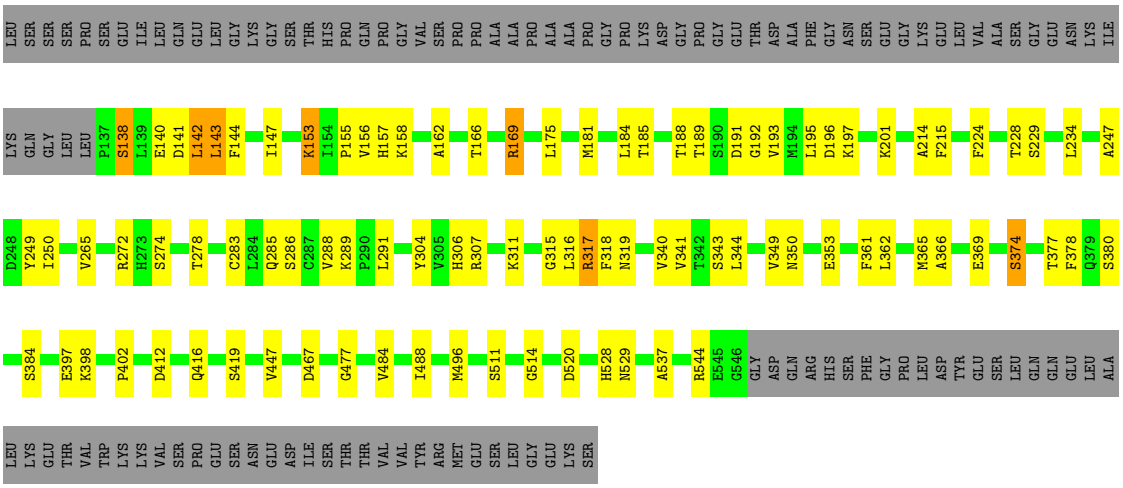
Chain E:





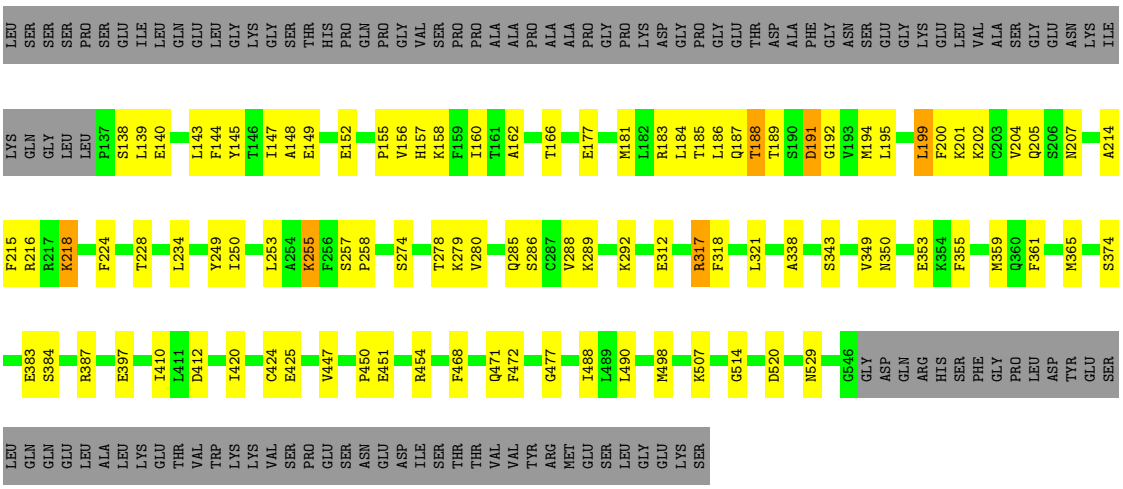
• Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain G:



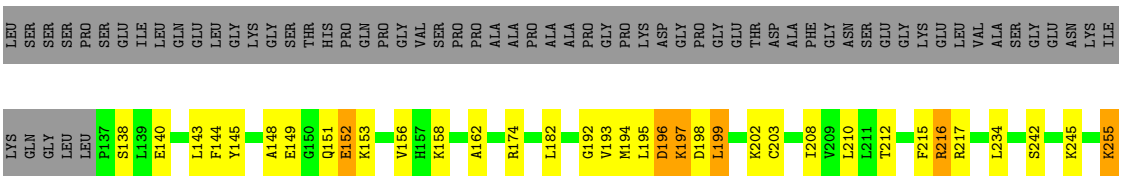
• Molecule 1: Glutaminase kidney isoform, mitochondrial

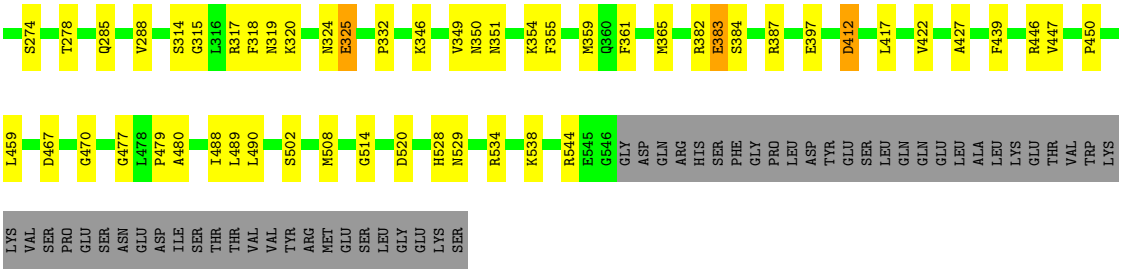
Chain F:



• Molecule 1: Glutaminase kidney isoform, mitochondrial

Chain H:




S274
T278
Q285
V288
S314
G315
L316
R317
F318
N319
K320
N324
E325
P332
K346
V349
N350
N351
K354
F355
M359
Q360
F361
M365
R382
E383
S384
R387
E397
D412
L417
V422
A427
F439
R446
V447
P450
L459
D467
G470
G477
L478
P479
A480
I488
L489
L490
S502
M508
G514
D520
H528
N529
R534
K538
R544
E545
G546
GLY
ASP
GLN
ARG
HIS
SER
PHE
GLY
PRO
LEU
ASP
TYR
GLU
SER
LEU
GLN
GLN
GLU
LEU
ALA
LEU
LYS
GLU
THR
VAL
TRP
LYS
LYS
VAL
SER
PRO
GLU
SER
ASN
GLU
ASP
ILE
SER
THR
THR
VAL
VAL
TYR
ARG
MET
GLU
SER
LEU
GLY
GLU
LYS
SER

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
$< I/\sigma(I) >$ [1]	1.75 (at 2.69Å)	Xtriage
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	96464 reflections (1.60%)	wwPDB-VP
Wilson B-factor (Å^2)	50.7	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 17.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.438 for h,-k,-l	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.53	0/3262	0.74	5/4403 (0.1%)
1	B	0.55	1/3266 (0.0%)	0.85	10/4408 (0.2%)
1	C	0.56	2/3266 (0.1%)	0.87	14/4408 (0.3%)
1	D	0.58	3/3266 (0.1%)	0.80	10/4408 (0.2%)
1	E	0.60	3/3262 (0.1%)	0.81	11/4403 (0.2%)
1	F	0.62	3/3266 (0.1%)	0.79	10/4408 (0.2%)
1	G	0.54	0/3266	0.87	16/4408 (0.4%)
1	H	0.58	4/3266 (0.1%)	0.82	11/4408 (0.2%)
All	All	0.57	16/26120 (0.1%)	0.82	87/35254 (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 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	255	LYS	CD-CE	13.03	1.83	1.51
1	E	317	ARG	CZ-NH2	12.27	1.49	1.33
1	E	317	ARG	CZ-NH1	-8.47	1.22	1.33
1	F	255	LYS	CE-NZ	7.72	1.68	1.49
1	B	317	ARG	CA-CB	7.70	1.70	1.53

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	139	LEU	CB-CG-CD1	-15.32	84.95	111.00
1	B	139	LEU	CA-CB-CG	14.91	149.58	115.30
1	G	143	LEU	CB-CG-CD2	-14.21	86.84	111.00
1	B	317	ARG	NE-CZ-NH2	-14.00	113.30	120.30
1	G	317	ARG	NE-CZ-NH1	12.13	126.37	120.30

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	78	0
1	B	3194	0	3170	65	0
1	C	3194	0	3170	66	0
1	D	3194	0	3170	76	0
1	E	3190	0	3165	69	0
1	F	3194	0	3170	70	0
1	G	3194	0	3170	66	0
1	H	3194	0	3170	73	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	525	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 10.

The worst 5 of 525 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:HB2	1:H:508:MET:CE	1.79	1.11

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%)	19	41
1	B	408/527 (77%)	392 (96%)	16 (4%)	0	100	100
1	C	408/527 (77%)	397 (97%)	10 (2%)	1 (0%)	44	67
1	D	408/527 (77%)	393 (96%)	13 (3%)	2 (0%)	25	50
1	E	407/527 (77%)	397 (98%)	9 (2%)	1 (0%)	44	67
1	F	408/527 (77%)	396 (97%)	11 (3%)	1 (0%)	44	67
1	G	408/527 (77%)	394 (97%)	13 (3%)	1 (0%)	44	67
1	H	408/527 (77%)	397 (97%)	10 (2%)	1 (0%)	44	67
All	All	3262/4216 (77%)	3159 (97%)	93 (3%)	10 (0%)	37	60

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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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%)	344 (98%)	9 (2%)	42	66
1	B	353/451 (78%)	343 (97%)	10 (3%)	38	63
1	C	353/451 (78%)	343 (97%)	10 (3%)	38	63
1	D	353/451 (78%)	341 (97%)	12 (3%)	32	57
1	E	353/451 (78%)	347 (98%)	6 (2%)	56	76
1	F	353/451 (78%)	343 (97%)	10 (3%)	38	63
1	G	353/451 (78%)	343 (97%)	10 (3%)	38	63
1	H	353/451 (78%)	341 (97%)	12 (3%)	32	57
All	All	2824/3608 (78%)	2745 (97%)	79 (3%)	38	63

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	138	SER
1	H	242	SER
1	F	218	LYS
1	F	451	GLU
1	H	412	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	347	GLN
1	D	252	GLN
1	E	360	GLN
1	F	471	GLN

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Mol	Chain	Res	Type
1	H	319	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	A	601	-	26,35,35	1.85	7 (26%)	28,49,49	2.48	13 (46%)
2	QA4	E	601	-	26,35,35	2.81	9 (34%)	28,49,49	3.10	11 (39%)
2	QA4	C	601	-	26,35,35	1.94	7 (26%)	28,49,49	2.00	8 (28%)
2	QA4	E	602	-	26,35,35	1.73	7 (26%)	28,49,49	1.90	5 (17%)

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	A	601	-	-	5/16/38/38	0/5/5/5
2	QA4	E	601	-	-	8/16/38/38	0/5/5/5
2	QA4	C	601	-	-	4/16/38/38	0/5/5/5
2	QA4	E	602	-	-	4/16/38/38	0/5/5/5

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	QA4	C25-N24	9.61	1.56	1.35
2	E	601	QA4	C11-N12	5.09	1.45	1.36
2	E	601	QA4	C13-N12	4.23	1.44	1.35
2	E	601	QA4	O07-C08	4.01	1.42	1.36
2	A	601	QA4	C13-N12	3.90	1.44	1.35

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	601	QA4	C14-C13-N12	7.39	123.76	114.62
2	E	601	QA4	C23-N24-C25	6.41	146.85	129.54
2	E	601	QA4	C04-C05-C06	6.04	116.86	110.32
2	E	601	QA4	O30-C25-C26	-5.63	113.31	121.54
2	A	601	QA4	C23-N24-C25	-5.38	115.01	129.54

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
2	C	601	QA4	S31-C20-N03-C02

There are no ring outliers.

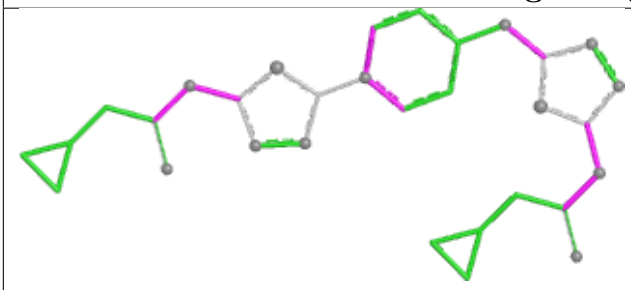
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	QA4	1	0
2	E	601	QA4	2	0

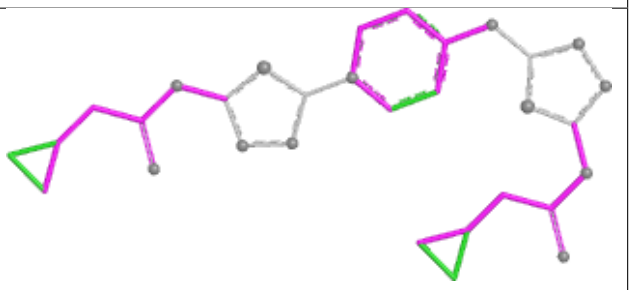
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 then 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.

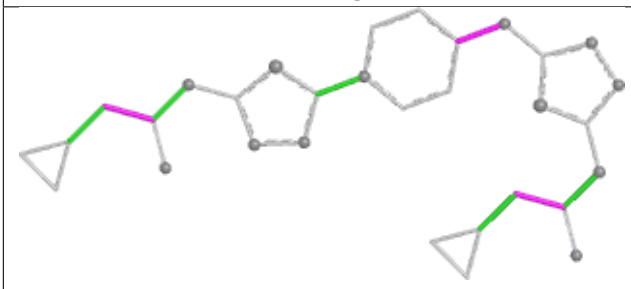
Ligand QA4 A 601



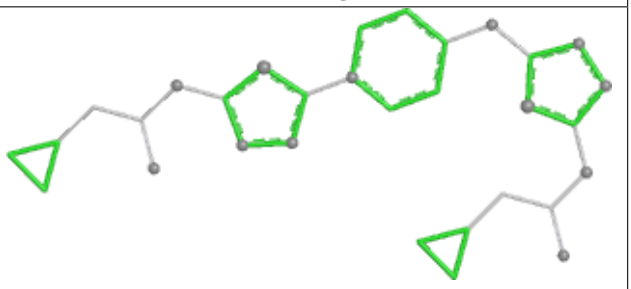
Bond lengths



Bond angles

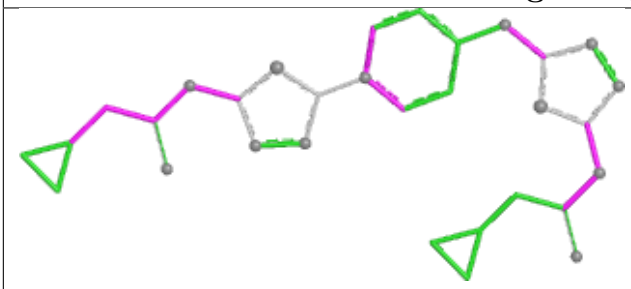


Torsions



Rings

Ligand QA4 E 601



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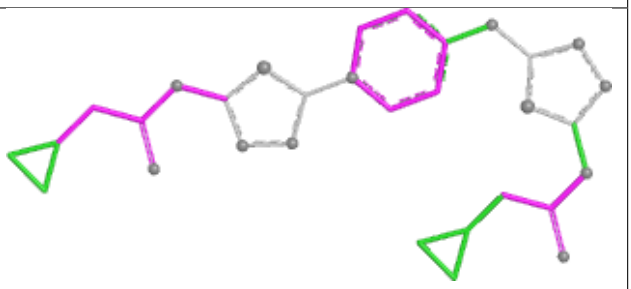
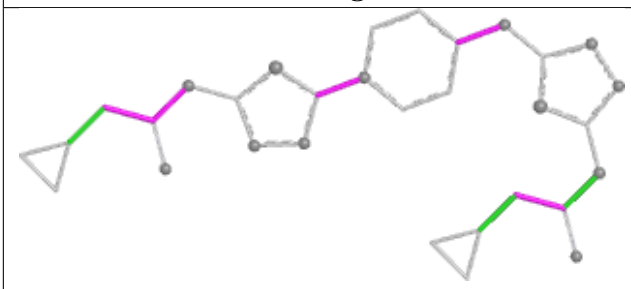


Bond angles



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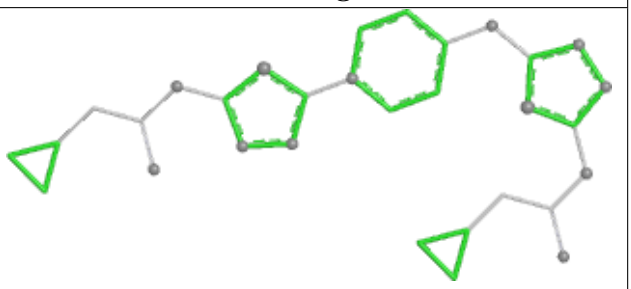
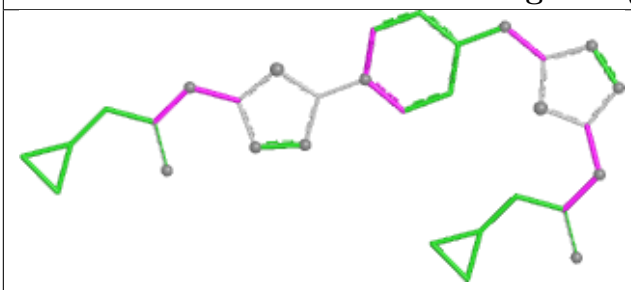


Rings

Ligand QA4 C 601



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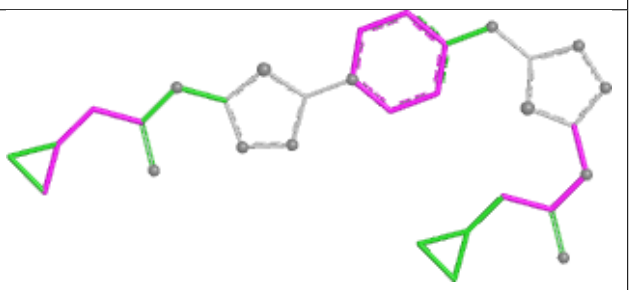
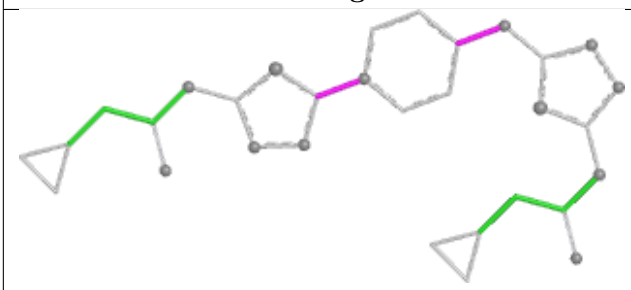


Bond angles



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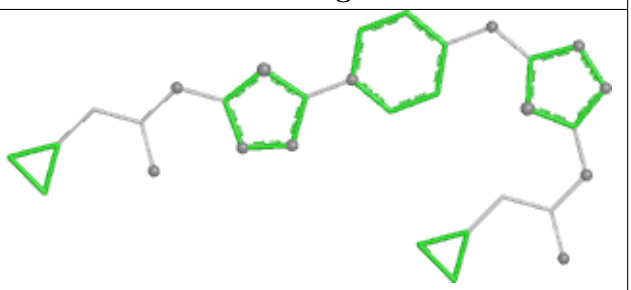
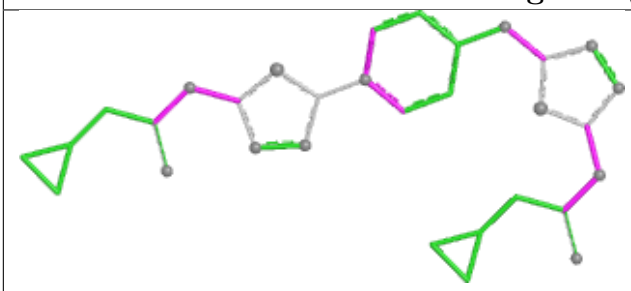
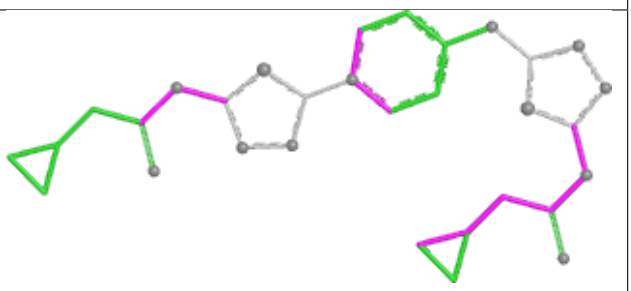


Rings

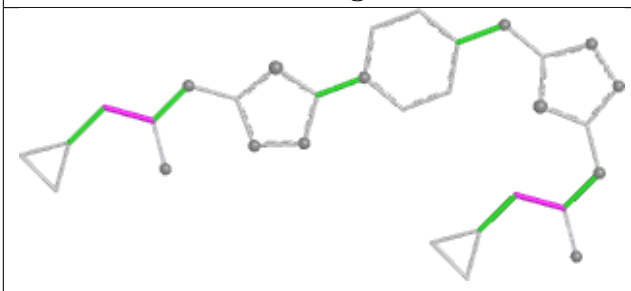
Ligand QA4 E 602



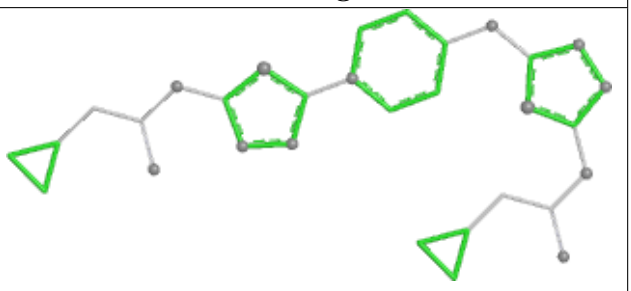
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	-1.74	0	100	100	25, 42, 100, 171	0
1	B	410/527 (77%)	-1.76	0	100	100	27, 41, 91, 152	0
1	C	410/527 (77%)	-1.75	0	100	100	27, 42, 96, 167	0
1	D	410/527 (77%)	-1.74	0	100	100	27, 41, 95, 155	0
1	E	409/527 (77%)	-1.77	0	100	100	26, 41, 88, 171	0
1	F	410/527 (77%)	-1.72	0	100	100	28, 42, 101, 162	0
1	G	410/527 (77%)	-1.74	0	100	100	28, 43, 95, 165	0
1	H	410/527 (77%)	-1.75	0	100	100	25, 42, 97, 175	0
All	All	3278/4216 (77%)	-1.75	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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

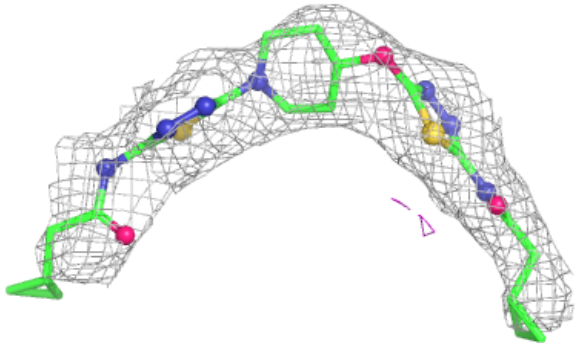
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

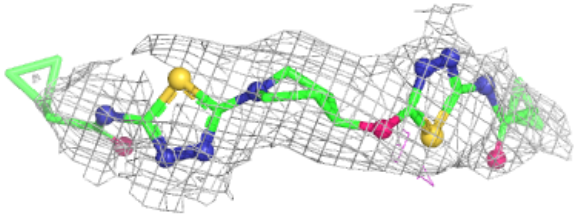
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	QA4	C	601	31/31	0.99	0.05	45,58,100,102	0
2	QA4	E	601	31/31	0.99	0.04	53,63,120,157	0
2	QA4	E	602	31/31	0.99	0.04	44,62,75,78	0
2	QA4	A	601	31/31	1.00	0.04	47,60,83,85	0

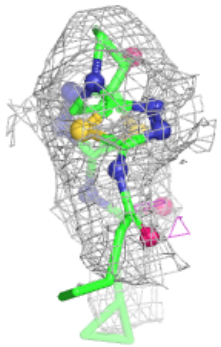
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around QA4 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)

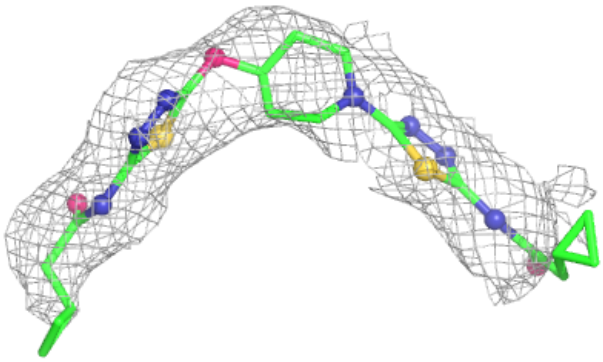


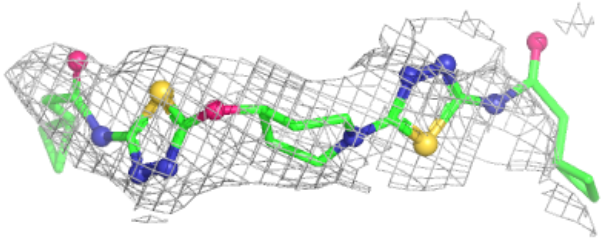


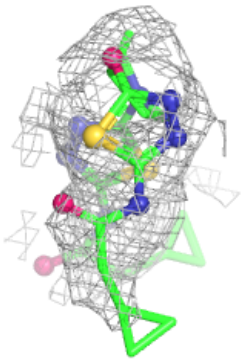


Electron density around QA4 E 601:

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

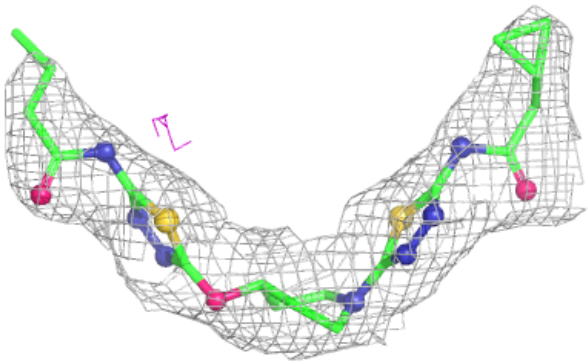


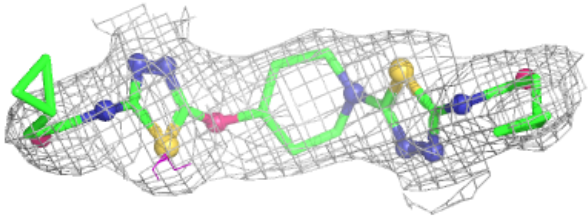


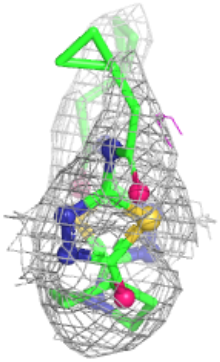


Electron density around QA4 E 602:

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

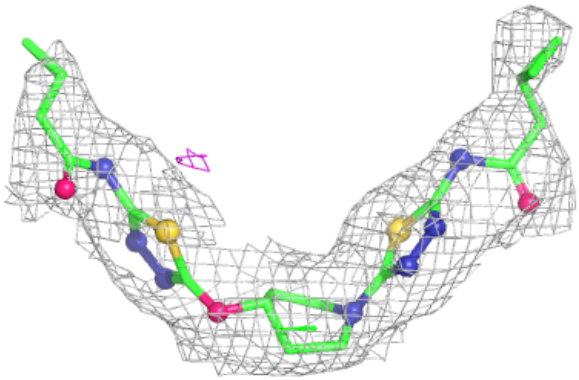


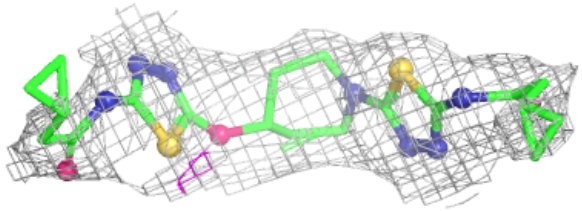


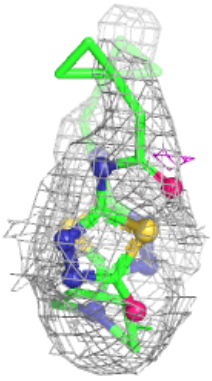


Electron density around QA4 A 601:

$2mF_o$-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

There are no such residues in this entry.