



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:00 pm BST

PDB ID : 5I94
Title : Crystal structure of human glutaminase C in complex with the inhibitor UPGL-00019
Authors : Huang, Q.; Cerione, R.
Deposited on : 2016-02-19
Resolution : 2.98 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

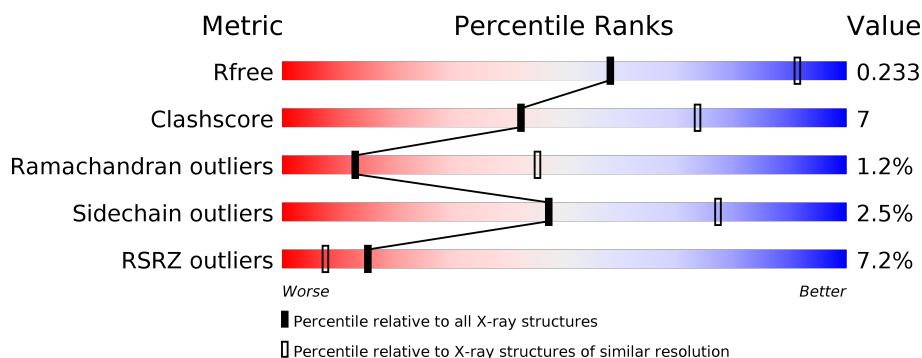
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 on 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	539	<div> <div>6%</div> <div> <div></div> <div>63%</div> <div>12%</div> <div>•</div> <div>24%</div> </div> </div>
1	B	539	<div> <div>4%</div> <div> <div></div> <div>60%</div> <div>15%</div> <div></div> <div>24%</div> </div> </div>
1	C	539	<div> <div>7%</div> <div> <div></div> <div>62%</div> <div>12%</div> <div>•</div> <div>24%</div> </div> </div>
1	D	539	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>12%</div> <div>•</div> <div>24%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12850 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	410	Total	C	N	O	S	1	0	0
			3194	2036	540	590	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			

There are 52 discrepancies between the modelled and reference sequences:

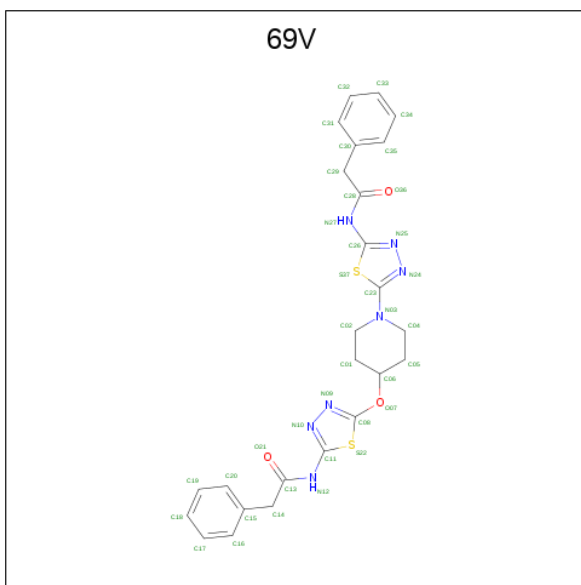
Chain	Residue	Modelled	Actual	Comment	Reference
A	59	MET	-	initiating methionine	UNP O94925
A	60	ARG	-	expression tag	UNP O94925
A	61	GLY	-	expression tag	UNP O94925
A	62	SER	-	expression tag	UNP O94925
A	63	HIS	-	expression tag	UNP O94925
A	64	HIS	-	expression tag	UNP O94925
A	65	HIS	-	expression tag	UNP O94925
A	66	HIS	-	expression tag	UNP O94925
A	67	HIS	-	expression tag	UNP O94925
A	68	HIS	-	expression tag	UNP O94925
A	69	GLY	-	expression tag	UNP O94925
A	70	SER	-	expression tag	UNP O94925
A	267	ALA	VAL	conflict	UNP O94925
B	59	MET	-	initiating methionine	UNP O94925
B	60	ARG	-	expression tag	UNP O94925
B	61	GLY	-	expression tag	UNP O94925
B	62	SER	-	expression tag	UNP O94925
B	63	HIS	-	expression tag	UNP O94925
B	64	HIS	-	expression tag	UNP O94925
B	65	HIS	-	expression tag	UNP O94925
B	66	HIS	-	expression tag	UNP O94925

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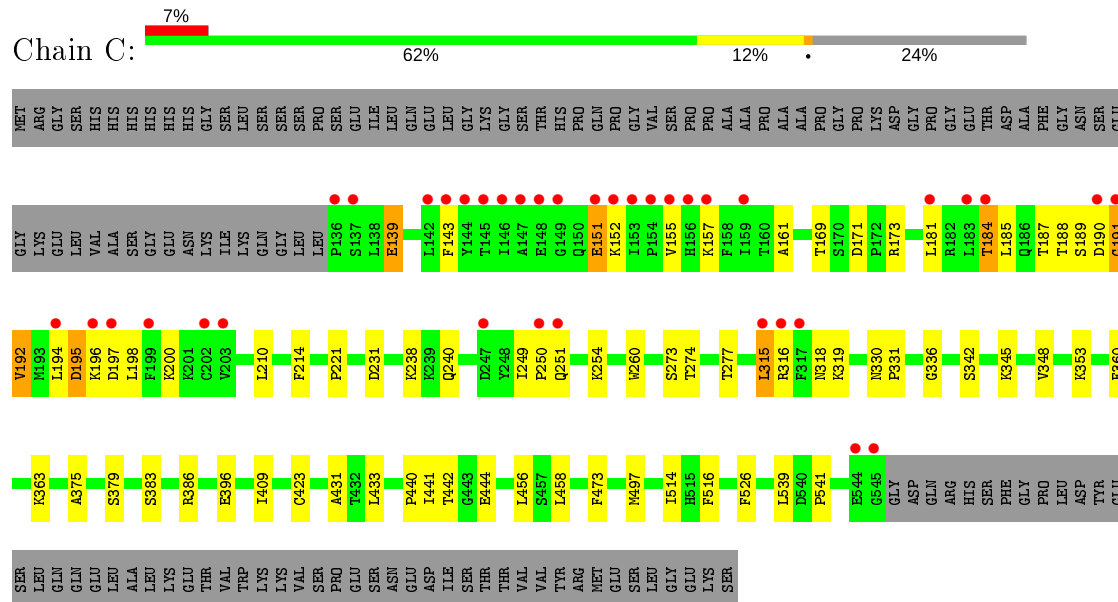
Chain	Residue	Modelled	Actual	Comment	Reference
B	67	HIS	-	expression tag	UNP O94925
B	68	HIS	-	expression tag	UNP O94925
B	69	GLY	-	expression tag	UNP O94925
B	70	SER	-	expression tag	UNP O94925
B	267	ALA	VAL	conflict	UNP O94925
C	59	MET	-	initiating methionine	UNP O94925
C	60	ARG	-	expression tag	UNP O94925
C	61	GLY	-	expression tag	UNP O94925
C	62	SER	-	expression tag	UNP O94925
C	63	HIS	-	expression tag	UNP O94925
C	64	HIS	-	expression tag	UNP O94925
C	65	HIS	-	expression tag	UNP O94925
C	66	HIS	-	expression tag	UNP O94925
C	67	HIS	-	expression tag	UNP O94925
C	68	HIS	-	expression tag	UNP O94925
C	69	GLY	-	expression tag	UNP O94925
C	70	SER	-	expression tag	UNP O94925
C	267	ALA	VAL	conflict	UNP O94925
D	59	MET	-	initiating methionine	UNP O94925
D	60	ARG	-	expression tag	UNP O94925
D	61	GLY	-	expression tag	UNP O94925
D	62	SER	-	expression tag	UNP O94925
D	63	HIS	-	expression tag	UNP O94925
D	64	HIS	-	expression tag	UNP O94925
D	65	HIS	-	expression tag	UNP O94925
D	66	HIS	-	expression tag	UNP O94925
D	67	HIS	-	expression tag	UNP O94925
D	68	HIS	-	expression tag	UNP O94925
D	69	GLY	-	expression tag	UNP O94925
D	70	SER	-	expression tag	UNP O94925
D	267	ALA	VAL	conflict	UNP O94925

- Molecule 2 is 2-phenyl-N-{5-[4-({5-[(phenylacetyl)amino]-1,3,4-thiadiazol-2-yl}oxy)piperidin-1-yl]-1,3,4-thiadiazol-2-yl}acetamide (three-letter code: 69V) (formula: C₂₅H₂₅N₇O₃S₂).

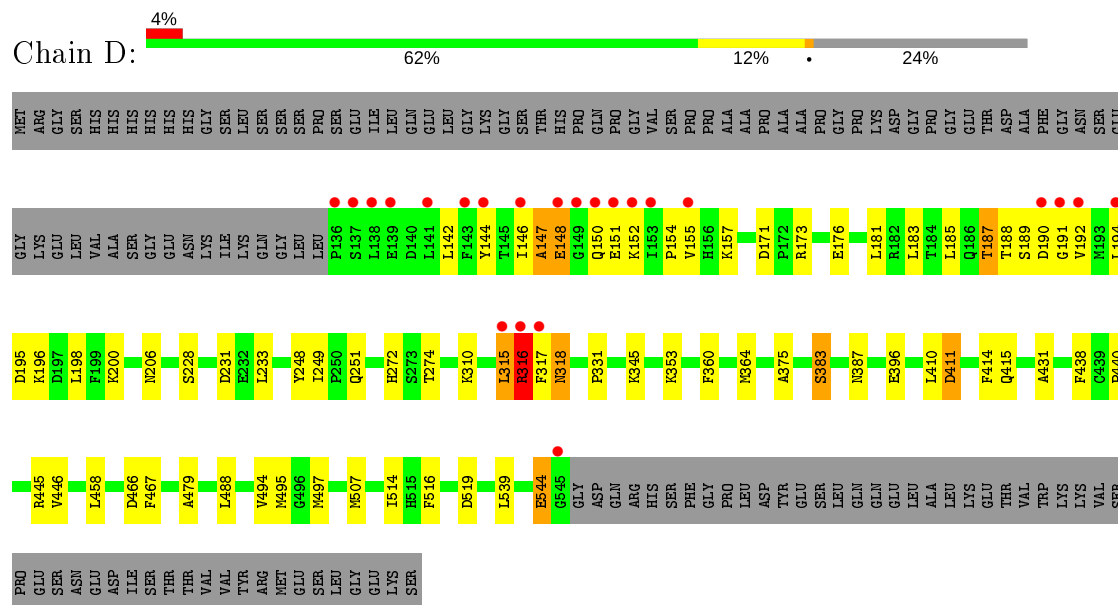


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 37	C 25	N 7	O 3	S 2	0	0
2	B	1	Total 37	C 25	N 7	O 3	S 2	0	0

- Molecule 1: Glutaminase kidney isoform, mitochondrial



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.44Å 137.79Å 175.75Å 90.00° 94.68° 90.00°	Depositor
Resolution (Å)	46.40 – 2.98 46.40 – 2.98	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.40-2.98) 98.8 (46.40-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.77 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.173 , 0.231 0.179 , 0.233	Depositor DCC
R_{free} test set	2013 reflections (4.26%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12850	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 69V

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	0/3266	0.62	0/4408
1	B	0.46	0/3266	0.64	0/4408
1	C	0.47	0/3266	0.63	0/4408
1	D	0.48	0/3266	0.64	3/4408 (0.1%)
All	All	0.47	0/13064	0.63	3/17632 (0.0%)

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	2
1	C	0	2
1	D	0	1
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	315	LEU	CA-CB-CG	6.48	130.21	115.30
1	D	316	ARG	CB-CG-CD	5.40	125.63	111.60
1	D	316	ARG	CA-CB-CG	-5.20	101.96	113.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	140	ASP	Peptide
1	B	189	SER	Peptide
1	C	187	THR	Peptide
1	C	315	LEU	Peptide
1	D	315	LEU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3194	0	3170	44	0
1	B	3194	0	3170	53	0
1	C	3194	0	3170	46	0
1	D	3194	0	3170	43	0
2	A	37	0	0	1	0
2	B	37	0	0	1	0
All	All	12850	0	12680	175	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 7.

All (175) 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:231:ASP:OD1	1:A:274:THR:HG21	1.13	1.27
1:B:231:ASP:OD1	1:B:274:THR:HG21	1.40	1.19
1:C:231:ASP:OD1	1:C:274:THR:HG21	1.49	1.12
1:D:231:ASP:OD1	1:D:274:THR:HG21	1.47	1.12
1:A:231:ASP:OD1	1:A:274:THR:CG2	2.06	1.02
1:B:249:ILE:HD12	1:B:379:SER:HB3	1.56	0.88
1:D:148:GLU:HB3	1:D:150:GLN:HB2	1.62	0.80
1:D:233:LEU:HD22	1:D:519:ASP:HB3	1.65	0.77
1:B:231:ASP:OD1	1:B:274:THR:CG2	2.29	0.76
1:B:273:SER:HB3	1:B:277:THR:HG21	1.67	0.76
1:C:194:LEU:HA	1:C:198:LEU:HD23	1.70	0.74
1:C:251:GLN:HA	1:C:254:LYS:HE3	1.68	0.74
1:B:194:LEU:HA	1:B:198:LEU:HD23	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ILE:HD12	1:A:379:SER:HB3	1.73	0.71
1:C:151:GLU:HG3	1:C:152:LYS:H	1.56	0.70
1:B:233:LEU:HD22	1:B:519:ASP:HB3	1.73	0.69
1:A:532:LEU:O	1:A:543:ARG:NH1	2.27	0.68
1:C:316:ARG:HD3	1:C:319:LYS:NZ	2.08	0.68
1:D:155:VAL:HG21	1:D:185:LEU:HD21	1.78	0.66
1:D:316:ARG:HG2	1:D:318:ASN:OD1	1.95	0.66
1:C:139:GLU:HG3	1:C:200:LYS:HG3	1.78	0.66
1:A:272:HIS:NE2	1:A:274:THR:HG23	2.10	0.65
1:B:140:ASP:HA	1:B:143:PHE:H	1.61	0.65
1:A:233:LEU:HD22	1:A:519:ASP:HB3	1.78	0.64
1:B:318:ASN:ND2	1:B:466:ASP:OD2	2.32	0.63
1:D:231:ASP:OD1	1:D:274:THR:CG2	2.37	0.61
1:D:316:ARG:HD3	1:D:466:ASP:OD2	2.01	0.61
1:D:467:PHE:HB2	1:D:507:MET:HG2	1.82	0.61
1:C:497:MET:HE1	1:C:516:PHE:CE1	2.35	0.60
1:A:272:HIS:NE2	1:A:274:THR:CG2	2.65	0.60
1:D:364:MET:HG2	1:D:446:VAL:HG11	1.84	0.59
1:D:154:PRO:HD2	1:D:157:LYS:HD2	1.84	0.57
1:D:316:ARG:HA	1:D:318:ASN:OD1	2.04	0.57
1:A:316:ARG:NH1	1:A:319:LYS:HD3	2.20	0.56
1:D:438:PHE:CE2	1:D:445:ARG:HB2	2.40	0.56
1:A:179:ASP:OD1	1:A:182:ARG:NH2	2.37	0.56
1:A:470:GLN:OE1	1:B:310:LYS:HE3	2.05	0.56
1:D:171:ASP:OD2	1:D:173:ARG:NH2	2.40	0.55
1:C:155:VAL:HG21	1:C:185:LEU:HD11	1.88	0.55
1:C:173:ARG:HD2	1:C:441:ILE:C	2.27	0.55
1:B:364:MET:HG3	1:B:446:VAL:HG11	1.89	0.54
1:D:147:ALA:O	1:D:148:GLU:HB2	2.07	0.54
1:A:460:HIS:HD1	1:B:529:TYR:HH	1.56	0.54
1:B:248:TYR:CE2	1:B:249:ILE:HG12	2.42	0.54
1:B:386:ARG:HB2	1:C:396:GLU:HG3	1.90	0.54
1:B:331:PRO:HD2	1:B:458:LEU:HD13	1.89	0.53
1:A:287:VAL:HG13	1:A:291:LYS:HE2	1.89	0.53
1:A:356:TYR:O	1:A:359:GLN:HG2	2.10	0.52
1:D:144:TYR:HA	1:D:147:ALA:HB2	1.92	0.52
1:A:248:TYR:CE2	1:A:249:ILE:HG12	2.45	0.51
1:A:378:GLN:O	1:A:381:ARG:HG2	2.10	0.51
1:A:383:SER:OG	1:A:383:SER:O	2.19	0.51
1:B:137:SER:O	1:B:141:LEU:HG	2.11	0.51
1:C:331:PRO:HD2	1:C:458:LEU:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:ASP:OD1	1:D:173:ARG:HD3	2.11	0.51
1:C:342:SER:HA	1:C:409:ILE:HD12	1.93	0.51
1:B:476:GLY:O	1:B:528:ASN:HB2	2.12	0.50
1:C:195:ASP:HB2	1:C:197:ASP:HB3	1.93	0.50
1:A:363:LYS:HD3	1:A:444:GLU:OE2	2.12	0.50
1:C:189:SER:C	1:C:191:GLY:H	2.14	0.50
1:D:431:ALA:HB1	1:D:440:PRO:HG2	1.92	0.50
1:D:497:MET:HE1	1:D:516:PHE:CE2	2.47	0.50
1:B:316:ARG:O	1:B:316:ARG:HG2	2.12	0.50
1:A:536:ALA:HB2	1:B:449:PRO:HG2	1.93	0.49
1:B:497:MET:HE1	1:B:516:PHE:HE2	1.77	0.49
1:D:411:ASP:O	1:D:415:GLN:HG3	2.13	0.49
1:A:324:GLU:OE2	1:B:316:ARG:HB3	2.12	0.49
1:A:292:TYR:OH	1:A:305:HIS:NE2	2.34	0.49
1:C:345:LYS:HB3	1:C:353:LYS:HG2	1.94	0.49
1:D:387:ASN:HD22	1:D:414:PHE:HE1	1.61	0.49
1:B:273:SER:O	1:B:274:THR:CG2	2.61	0.49
1:A:140:ASP:O	1:A:143:PHE:HB3	2.13	0.49
1:A:393:TYR:OH	2:A:601:69V:S22	2.64	0.49
1:D:233:LEU:CD2	1:D:519:ASP:HB3	2.41	0.48
1:D:194:LEU:HA	1:D:198:LEU:HD23	1.96	0.48
1:A:479:ALA:HB2	1:A:489:LEU:HD12	1.96	0.48
1:D:142:LEU:HD11	1:D:146:ILE:HD11	1.96	0.48
1:B:154:PRO:HD2	1:B:157:LYS:HD2	1.95	0.48
1:C:363:LYS:HD3	1:C:444:GLU:OE2	2.14	0.48
1:D:248:TYR:CD1	1:D:249:ILE:HG23	2.49	0.47
1:D:345:LYS:HB3	1:D:353:LYS:HG2	1.94	0.47
1:B:152:LYS:HB2	1:B:193:MET:HE3	1.97	0.47
1:A:151:GLU:OE1	1:A:151:GLU:N	2.47	0.47
1:B:153:ILE:HG23	1:B:157:LYS:HD3	1.97	0.47
1:C:171:ASP:OD1	1:C:173:ARG:HD3	2.14	0.47
1:B:171:ASP:OD1	1:B:173:ARG:HD3	2.15	0.47
1:A:386:ARG:HB2	1:D:396:GLU:HG3	1.96	0.47
1:C:316:ARG:HD3	1:C:319:LYS:HZ2	1.78	0.46
1:D:191:GLY:HA3	1:D:192:VAL:HA	1.54	0.46
1:A:273:SER:HB3	1:A:277:THR:HG21	1.96	0.46
1:A:200:LYS:O	1:A:204:GLN:HG3	2.15	0.46
1:A:277:THR:O	1:A:424:GLU:HG3	2.15	0.46
1:B:315:LEU:H	1:B:315:LEU:HD12	1.80	0.46
1:B:231:ASP:O	1:B:234:TYR:HB3	2.16	0.46
1:D:152:LYS:HG2	1:D:195:ASP:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ALA:HB1	1:C:214:PHE:HE1	1.81	0.46
1:C:151:GLU:CG	1:C:152:LYS:H	2.26	0.45
1:A:194:LEU:HD23	1:A:198:LEU:HG	1.98	0.45
1:B:148:GLU:HB3	1:B:149:GLY:H	1.49	0.45
1:B:264:VAL:HG22	1:B:497:MET:HG2	1.98	0.45
1:D:544:GLU:N	1:D:544:GLU:OE1	2.48	0.45
1:A:146:ILE:HB	1:A:153:ILE:HD13	1.99	0.45
1:B:497:MET:HE1	1:B:516:PHE:CE2	2.51	0.45
1:D:410:LEU:HD23	1:D:410:LEU:HA	1.74	0.45
1:D:494:VAL:HG12	1:D:495:MET:HG2	1.99	0.45
1:B:284:GLN:O	1:B:287:VAL:HG12	2.17	0.45
1:C:238:LYS:HG3	1:C:260:TRP:HD1	1.81	0.45
1:A:171:ASP:OD1	1:A:173:ARG:HD3	2.17	0.45
1:C:441:ILE:HG13	1:C:442:THR:HG23	1.99	0.45
1:C:497:MET:HE1	1:C:516:PHE:HE1	1.80	0.45
1:B:201:LYS:HA	1:B:204:GLN:NE2	2.32	0.44
1:D:497:MET:HE1	1:D:516:PHE:HE2	1.82	0.44
1:A:152:LYS:HE3	1:A:193:MET:HB3	1.99	0.44
1:A:529:TYR:HH	1:B:460:HIS:HD1	1.62	0.44
1:C:348:VAL:O	1:C:353:LYS:HE3	2.18	0.44
1:B:161:ALA:HB1	1:B:214:PHE:HE1	1.82	0.44
1:C:251:GLN:HE21	1:C:375:ALA:HB1	1.82	0.44
1:C:195:ASP:HB2	1:C:198:LEU:H	1.83	0.44
1:C:315:LEU:HD12	1:C:315:LEU:HA	1.51	0.44
1:B:319:LYS:HB3	2:B:601:69V:N10	2.33	0.44
1:D:331:PRO:HD2	1:D:458:LEU:HD13	1.98	0.44
1:D:187:THR:O	1:D:189:SER:N	2.50	0.44
1:B:142:LEU:O	1:B:145:THR:HB	2.18	0.44
1:C:189:SER:O	1:C:191:GLY:N	2.50	0.44
1:C:473:PHE:CD2	1:D:310:LYS:HD2	2.53	0.44
1:B:191:GLY:HA3	1:B:192:VAL:HA	1.55	0.43
1:A:152:LYS:HB3	1:A:193:MET:HG3	2.00	0.43
1:A:530:ASP:OD1	1:B:453:ARG:HD3	2.18	0.43
1:A:348:VAL:O	1:A:353:LYS:HE3	2.18	0.43
1:B:350:ASN:ND2	1:B:408:GLY:O	2.45	0.43
1:B:396:GLU:HG3	1:C:386:ARG:HB2	1.99	0.43
1:D:272:HIS:NE2	1:D:274:THR:CG2	2.81	0.43
1:C:189:SER:C	1:C:191:GLY:N	2.72	0.43
1:B:363:LYS:HB3	1:B:446:VAL:HG22	2.01	0.43
1:B:479:ALA:HA	1:B:488:LEU:O	2.19	0.43
1:B:249:ILE:HG22	1:B:251:GLN:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:526:PHE:CZ	1:C:541:PRO:HG2	2.54	0.43
1:B:173:ARG:HD2	1:B:441:ILE:C	2.40	0.42
1:C:514:ILE:HA	1:C:514:ILE:HD13	1.89	0.42
1:C:191:GLY:HA3	1:C:192:VAL:HA	1.76	0.42
1:B:376:THR:O	1:B:380:GLU:HB2	2.19	0.42
1:C:157:LYS:HA	1:C:157:LYS:HD2	1.82	0.42
1:C:433:LEU:HB3	1:C:456:LEU:HD21	2.00	0.42
1:A:173:ARG:HD2	1:A:441:ILE:C	2.39	0.42
1:C:277:THR:HA	1:C:423:CYS:HB2	2.01	0.42
1:D:142:LEU:O	1:D:146:ILE:HG13	2.20	0.42
1:D:176:GLU:HG2	1:D:206:ASN:HD21	1.84	0.42
1:A:219:VAL:HG13	1:A:220:ILE:HG13	2.01	0.42
1:B:208:VAL:O	1:B:212:GLN:HG3	2.19	0.42
1:C:184:THR:HG22	1:C:185:LEU:HD23	2.02	0.42
1:A:191:GLY:HA3	1:A:192:VAL:HA	1.50	0.42
1:B:140:ASP:HB2	1:B:143:PHE:HB3	2.01	0.41
1:C:210:LEU:O	1:C:214:PHE:HD2	2.03	0.41
1:D:251:GLN:HE21	1:D:375:ALA:HB1	1.85	0.41
1:D:514:ILE:HA	1:D:514:ILE:HD13	1.80	0.41
1:B:266:THR:CG2	1:B:270:GLN:HB2	2.50	0.41
1:C:143:PHE:CE2	1:C:196:LYS:HB2	2.55	0.41
1:A:152:LYS:HB3	1:A:193:MET:CG	2.50	0.41
1:B:217:LYS:HA	1:B:217:LYS:HD3	1.85	0.41
1:C:273:SER:O	1:C:274:THR:CG2	2.67	0.41
1:B:333:VAL:HG23	1:B:336:GLY:H	1.85	0.41
1:A:184:THR:C	1:A:186:GLN:H	2.23	0.41
1:C:181:LEU:O	1:C:185:LEU:HG	2.20	0.41
1:A:277:THR:HA	1:A:423:CYS:HB2	2.03	0.41
1:B:223:PHE:O	1:B:227:THR:HG23	2.20	0.41
1:D:181:LEU:O	1:D:185:LEU:HG	2.21	0.41
1:B:273:SER:O	1:B:274:THR:HG23	2.22	0.40
1:D:479:ALA:HA	1:D:488:LEU:O	2.21	0.40
1:A:453:ARG:HD2	1:B:527:HIS:CG	2.56	0.40
1:D:183:LEU:HD12	1:D:183:LEU:HA	1.93	0.40
1:A:359:GLN:HG3	1:A:360:PHE:N	2.27	0.40
1:C:249:ILE:HA	1:C:250:PRO:HD2	1.87	0.40
1:C:330:ASN:O	1:C:336:GLY:HA3	2.22	0.40
1:C:249:ILE:HD13	1:C:379:SER:HB3	2.03	0.40
1:C:431:ALA:HB1	1:C:440:PRO:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	408/539 (76%)	385 (94%)	20 (5%)	3 (1%)	22	58
1	B	408/539 (76%)	369 (90%)	35 (9%)	4 (1%)	15	50
1	C	408/539 (76%)	373 (91%)	31 (8%)	4 (1%)	15	50
1	D	408/539 (76%)	379 (93%)	20 (5%)	9 (2%)	6	29
All	All	1632/2156 (76%)	1506 (92%)	106 (6%)	20 (1%)	13	45

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	LEU
1	B	190	ASP
1	B	544	GLU
1	C	190	ASP
1	D	147	ALA
1	D	148	GLU
1	D	187	THR
1	B	315	LEU
1	C	151	GLU
1	C	191	GLY
1	D	190	ASP
1	D	383	SER
1	D	196	LYS
1	D	316	ARG
1	D	544	GLU
1	A	185	LEU
1	A	318	ASN
1	B	150	GLN
1	D	188	THR
1	C	221	PRO

5.3.2 Protein sidechains ⓘ

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	353/461 (77%)	344 (98%)	9 (2%)	47	77
1	B	353/461 (77%)	346 (98%)	7 (2%)	55	81
1	C	353/461 (77%)	342 (97%)	11 (3%)	40	73
1	D	353/461 (77%)	344 (98%)	9 (2%)	47	77
All	All	1412/1844 (77%)	1376 (98%)	36 (2%)	47	77

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	LEU
1	A	240	GLN
1	A	285	SER
1	A	318	ASN
1	A	319	LYS
1	A	359	GLN
1	A	360	PHE
1	A	383	SER
1	A	411	ASP
1	B	140	ASP
1	B	151	GLU
1	B	177	CYS
1	B	197	ASP
1	B	285	SER
1	B	360	PHE
1	B	528	ASN
1	C	139	GLU
1	C	169	THR
1	C	184	THR
1	C	188	THR
1	C	192	VAL
1	C	195	ASP
1	C	240	GLN
1	C	318	ASN

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Mol	Chain	Res	Type
1	C	360	PHE
1	C	383	SER
1	C	539	LEU
1	D	151	GLU
1	D	200	LYS
1	D	228	SER
1	D	317	PHE
1	D	318	ASN
1	D	360	PHE
1	D	383	SER
1	D	411	ASP
1	D	539	LEU

Some 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 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	69V	A	601	-	33,41,41	2.02	8 (24%)	34,55,55	2.05	9 (26%)
2	69V	B	601	-	33,41,41	2.02	9 (27%)	34,55,55	1.99	7 (20%)

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	69V	A	601	-	-	8/16/34/34	0/5/5/5
2	69V	B	601	-	-	4/16/34/34	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	69V	C23-N03	7.07	1.43	1.32
2	B	601	69V	C23-N03	6.33	1.42	1.32
2	B	601	69V	O07-C08	4.45	1.42	1.36
2	A	601	69V	O07-C08	4.09	1.41	1.36
2	A	601	69V	C11-N12	4.05	1.43	1.36
2	B	601	69V	C11-N12	3.65	1.43	1.36
2	B	601	69V	C13-N12	3.51	1.43	1.35
2	B	601	69V	C02-N03	-3.30	1.41	1.46
2	A	601	69V	C13-N12	3.20	1.42	1.35
2	B	601	69V	C28-N27	3.16	1.42	1.35
2	A	601	69V	C04-N03	-3.04	1.42	1.46
2	B	601	69V	C04-N03	-3.03	1.42	1.46
2	B	601	69V	C26-N27	3.00	1.42	1.36
2	A	601	69V	C02-N03	-2.95	1.42	1.46
2	A	601	69V	C28-N27	2.85	1.42	1.35
2	A	601	69V	C26-N27	2.71	1.41	1.36
2	B	601	69V	N10-N09	-2.04	1.33	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	69V	C04-N03-C02	7.23	127.48	111.52
2	A	601	69V	C04-N03-C02	6.46	125.78	111.52
2	B	601	69V	C11-N12-C13	-4.87	116.40	129.54
2	B	601	69V	C14-C13-N12	4.00	123.03	114.77
2	A	601	69V	C02-C01-C06	3.70	114.39	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	69V	C26-N27-C28	-3.48	120.14	129.54
2	A	601	69V	O21-C13-N12	-3.23	117.74	123.63
2	A	601	69V	C05-C06-C01	-2.88	106.18	111.74
2	A	601	69V	C29-C28-N27	2.85	120.65	114.77
2	A	601	69V	C14-C13-N12	2.69	120.32	114.77
2	A	601	69V	C04-C05-C06	2.56	113.13	110.32
2	B	601	69V	O21-C13-C14	-2.50	116.33	122.03
2	B	601	69V	C04-C05-C06	2.48	113.05	110.32
2	A	601	69V	C15-C14-C13	2.40	119.70	112.57
2	B	601	69V	C05-C06-C01	-2.18	107.53	111.74
2	B	601	69V	C26-N27-C28	-2.14	123.75	129.54

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	69V	S37-C23-N03-C02
2	A	601	69V	S37-C23-N03-C04
2	B	601	69V	S37-C23-N03-C02
2	B	601	69V	S37-C23-N03-C04
2	A	601	69V	C13-C14-C15-C16
2	B	601	69V	O36-C28-C29-C30
2	A	601	69V	C13-C14-C15-C20
2	B	601	69V	N27-C28-C29-C30
2	A	601	69V	C01-C06-O07-C08
2	A	601	69V	C05-C06-O07-C08
2	A	601	69V	C14-C13-N12-C11
2	A	601	69V	O21-C13-N12-C11

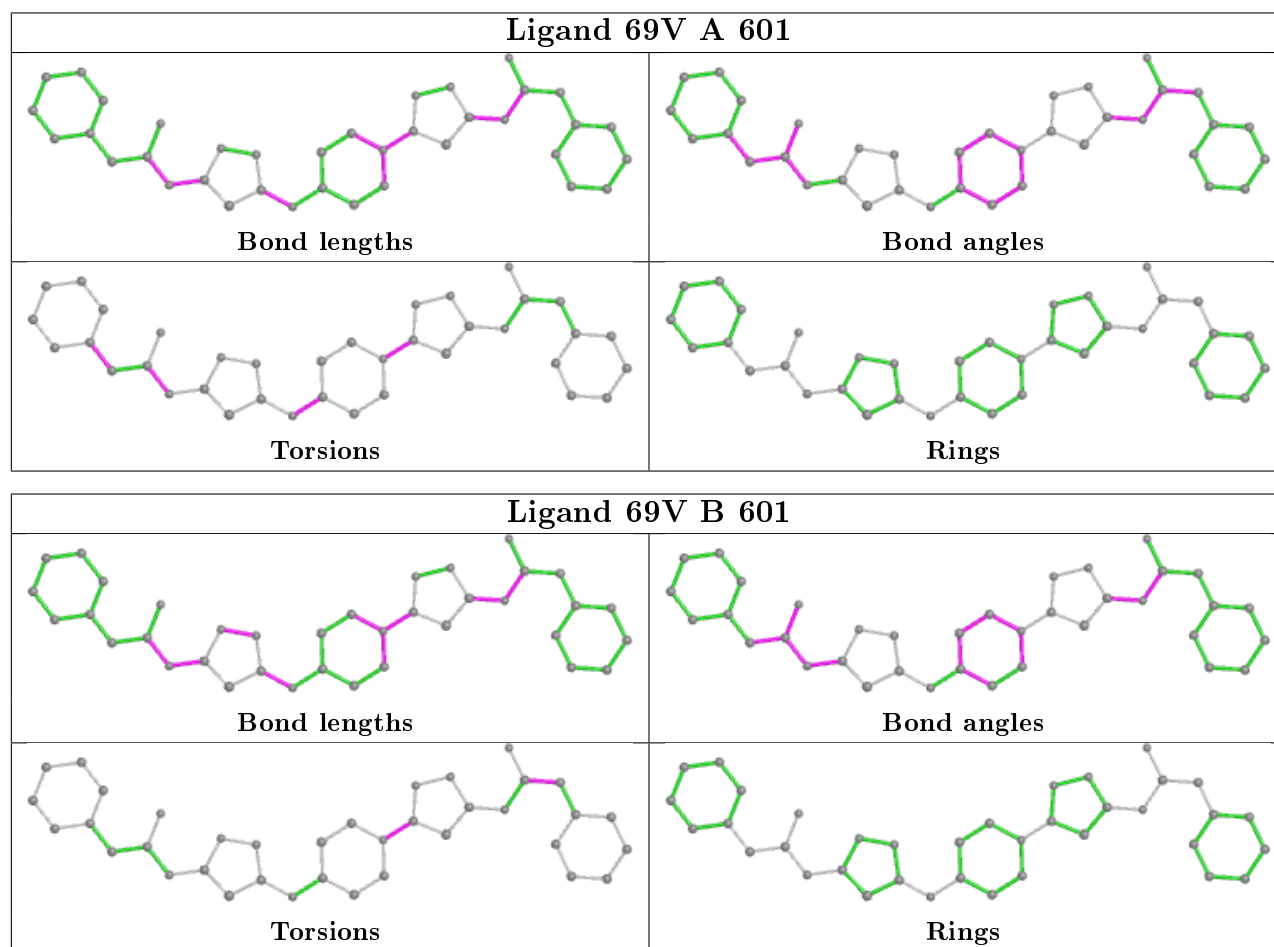
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	69V	1	0
2	B	601	69V	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

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	410/539 (76%)	0.14	35 (8%) 10 5	19, 29, 78, 100	0
1	B	410/539 (76%)	0.04	23 (5%) 24 13	18, 31, 73, 92	0
1	C	410/539 (76%)	0.14	37 (9%) 9 5	16, 28, 78, 97	0
1	D	410/539 (76%)	0.01	23 (5%) 24 13	17, 30, 74, 95	0
All	All	1640/2156 (76%)	0.08	118 (7%) 15 8	16, 30, 77, 100	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	149	GLY	6.8
1	A	545	GLY	6.5
1	D	136	PRO	5.3
1	A	136	PRO	5.3
1	B	251	GLN	5.2
1	D	190	ASP	5.0
1	D	315	LEU	4.8
1	A	149	GLY	4.6
1	A	188	THR	4.6
1	A	152	LYS	4.6
1	B	316	ARG	4.6
1	A	151	GLU	4.5
1	C	148	GLU	4.5
1	B	250	PRO	4.4
1	C	545	GLY	4.3
1	A	148	GLU	4.3
1	D	316	ARG	4.2
1	C	145	THR	4.2
1	D	148	GLU	4.1
1	C	144	TYR	4.1
1	D	151	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	191	GLY	4.0
1	C	143	PHE	3.9
1	A	144	TYR	3.8
1	A	145	THR	3.8
1	C	142	LEU	3.7
1	C	147	ALA	3.7
1	C	251	GLN	3.7
1	C	315	LEU	3.7
1	B	149	GLY	3.7
1	C	184	THR	3.7
1	C	194	LEU	3.6
1	C	149	GLY	3.6
1	C	191	GLY	3.6
1	C	316	ARG	3.5
1	A	194	LEU	3.5
1	A	192	VAL	3.4
1	B	545	GLY	3.4
1	A	199	PHE	3.4
1	D	152	LYS	3.4
1	A	155	VAL	3.4
1	B	136	PRO	3.4
1	C	152	LYS	3.3
1	C	197	ASP	3.2
1	C	153	ILE	3.2
1	B	190	ASP	3.2
1	A	196	LYS	3.2
1	A	141	LEU	3.2
1	A	315	LEU	3.2
1	A	184	THR	3.1
1	B	199	PHE	3.1
1	B	248	TYR	3.1
1	B	192	VAL	3.0
1	C	196	LYS	3.0
1	C	151	GLU	3.0
1	B	255	PHE	3.0
1	C	250	PRO	3.0
1	D	144	TYR	3.0
1	B	144	TYR	3.0
1	A	137	SER	2.9
1	A	316	ARG	2.9
1	C	136	PRO	2.9
1	A	193	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	315	LEU	2.8
1	B	155	VAL	2.8
1	B	140	ASP	2.7
1	D	545	GLY	2.7
1	A	187	THR	2.7
1	A	154	PRO	2.7
1	C	190	ASP	2.7
1	A	544	GLU	2.7
1	A	142	LEU	2.7
1	D	317	PHE	2.7
1	A	143	PHE	2.6
1	A	153	ILE	2.6
1	C	155	VAL	2.6
1	A	211	THR	2.5
1	D	143	PHE	2.5
1	D	192	VAL	2.5
1	C	146	ILE	2.5
1	C	317	PHE	2.5
1	A	197	ASP	2.5
1	D	138	LEU	2.5
1	C	199	PHE	2.5
1	C	202	CYS	2.5
1	A	207	ILE	2.5
1	A	138	LEU	2.4
1	B	147	ALA	2.4
1	B	143	PHE	2.3
1	D	194	LEU	2.3
1	B	191	GLY	2.3
1	D	141	LEU	2.3
1	C	183	LEU	2.3
1	C	157	LYS	2.3
1	B	203	VAL	2.2
1	C	203	VAL	2.2
1	A	146	ILE	2.2
1	A	190	ASP	2.2
1	D	153	ILE	2.2
1	C	544	GLU	2.2
1	D	150	GLN	2.2
1	B	145	THR	2.2
1	D	146	ILE	2.2
1	C	247	ASP	2.2
1	C	154	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	215	ARG	2.2
1	B	151	GLU	2.1
1	B	148	GLU	2.1
1	C	137	SER	2.1
1	D	137	SER	2.1
1	C	181	LEU	2.1
1	D	155	VAL	2.1
1	C	156	HIS	2.1
1	D	139	GLU	2.1
1	C	159	ILE	2.0
1	A	186	GLN	2.0
1	B	249	ILE	2.0
1	A	147	ALA	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 carbohydrates in this entry.

6.4 Ligands [i](#)

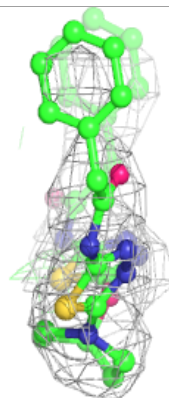
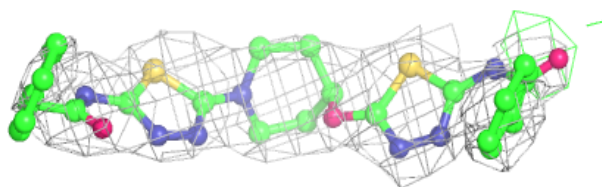
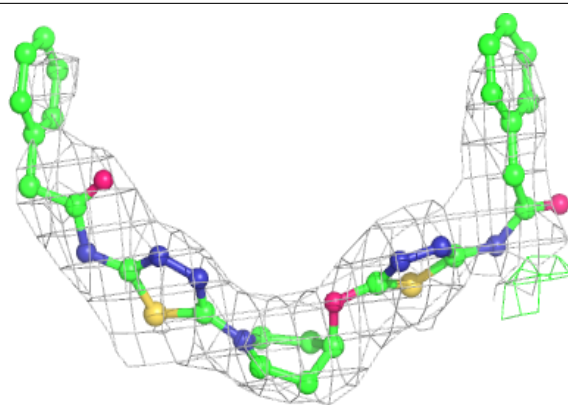
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	69V	A	601	37/37	0.92	0.28	45,65,81,85	0
2	69V	B	601	37/37	0.92	0.27	50,63,81,82	0

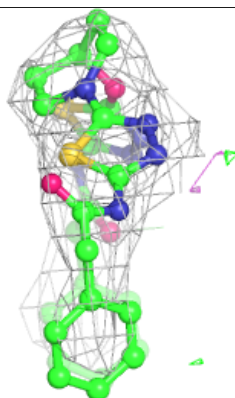
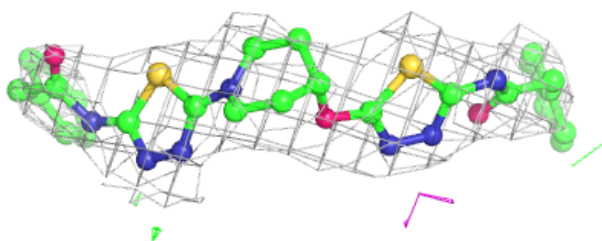
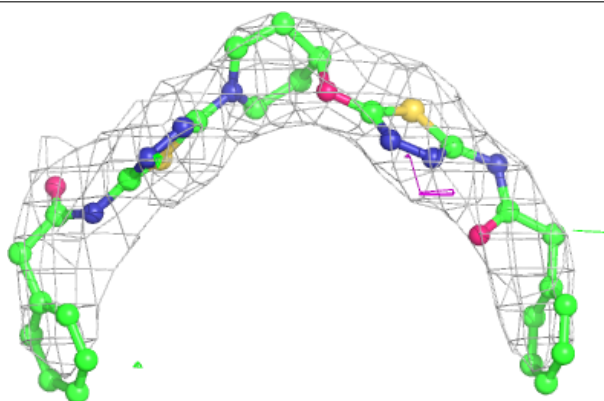
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 69V A 601:

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

**Electron density around 69V B 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.