



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:47 PM UTC

PDB ID : 8JUE / pdb_00008jue
Title : Crystal structure of glutaminase C in complex with compound 11
Authors : Wang, X.; Hanyu, S.; Tingting, D.
Deposited on : 2023-06-26
Resolution : 2.39 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 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

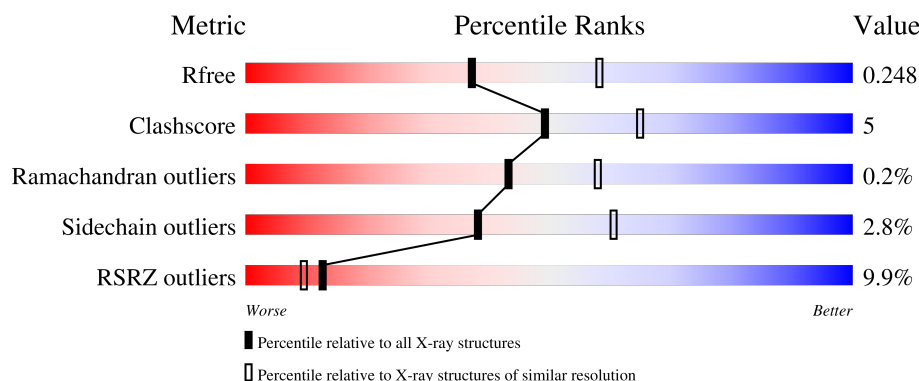
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	533	
1	B	533	
1	C	533	
1	D	533	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12864 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	401	Total	C	N	O	S	0	0	0
			3138	2005	530	575	28			
1	B	403	Total	C	N	O	S	0	0	0
			3155	2015	533	579	28			
1	C	393	Total	C	N	O	S	0	0	0
			3076	1962	521	565	28			
1	D	392	Total	C	N	O	S	0	0	0
			3067	1958	519	562	28			

There are 32 discrepancies between the modelled and reference sequences:

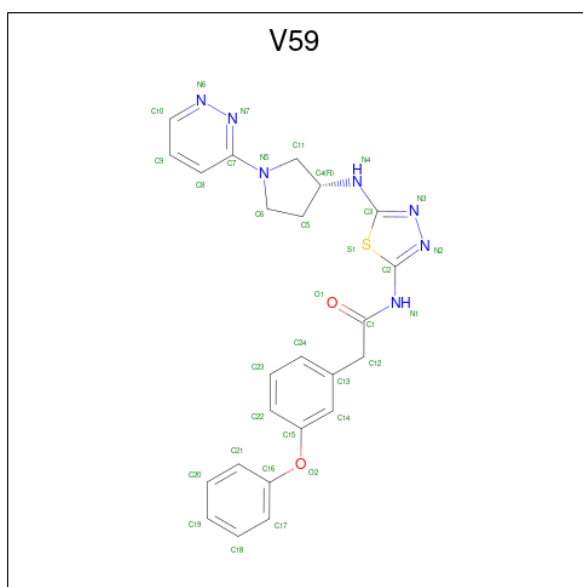
Chain	Residue	Modelled	Actual	Comment	Reference
A	63	MET	-	initiating methionine	UNP O94925
A	64	GLY	-	expression tag	UNP O94925
A	65	HIS	-	expression tag	UNP O94925
A	66	HIS	-	expression tag	UNP O94925
A	67	HIS	-	expression tag	UNP O94925
A	68	HIS	-	expression tag	UNP O94925
A	69	HIS	-	expression tag	UNP O94925
A	70	HIS	-	expression tag	UNP O94925
B	63	MET	-	initiating methionine	UNP O94925
B	64	GLY	-	expression tag	UNP O94925
B	65	HIS	-	expression tag	UNP O94925
B	66	HIS	-	expression tag	UNP O94925
B	67	HIS	-	expression tag	UNP O94925
B	68	HIS	-	expression tag	UNP O94925
B	69	HIS	-	expression tag	UNP O94925
B	70	HIS	-	expression tag	UNP O94925
C	63	MET	-	initiating methionine	UNP O94925
C	64	GLY	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	68	HIS	-	expression tag	UNP O94925
C	69	HIS	-	expression tag	UNP O94925
C	70	HIS	-	expression tag	UNP O94925
D	63	MET	-	initiating methionine	UNP O94925
D	64	GLY	-	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	HIS	-	expression tag	UNP O94925
D	70	HIS	-	expression tag	UNP O94925

- Molecule 2 is 2-(3-phenoxyphenyl)-N-[5-[[[(3R)-1-pyridazin-3-ylpyrrolidin-3-yl]amino]-1,3,4-t hiadiazol-2-yl]ethanamide (CCD ID: V59) (formula: C₂₄H₂₃N₇O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			34	24	7	2	1		
2	C	1	Total	C	N	O	S	0	0
			34	24	7	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	94	Total	O	0	0
			94	94		

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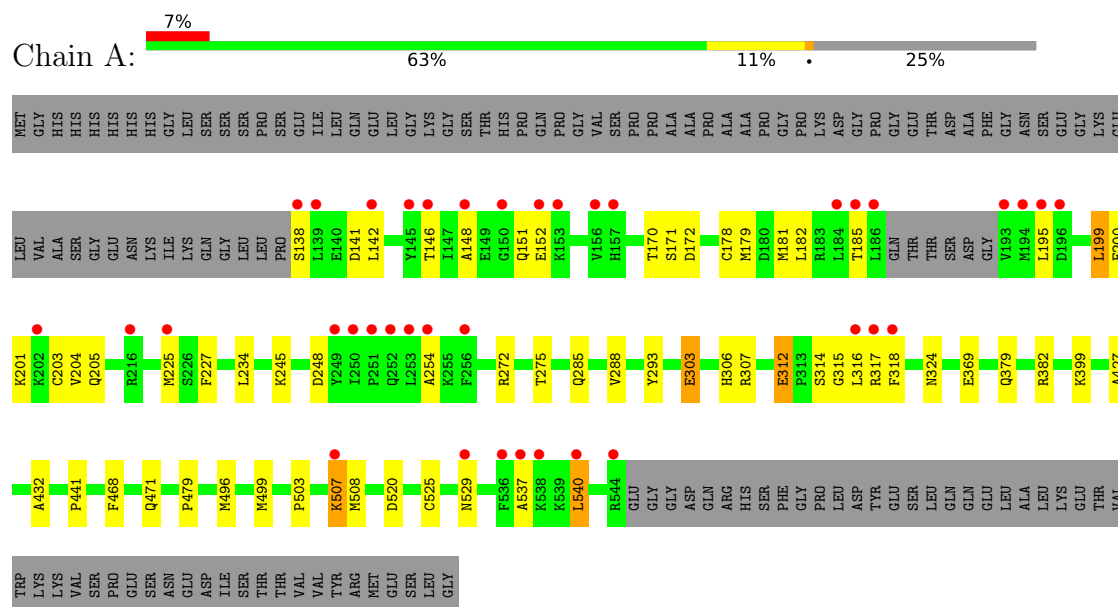
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	87	Total 87	O 87	0	0
3	C	85	Total 85	O 85	0	0
3	D	94	Total 94	O 94	0	0

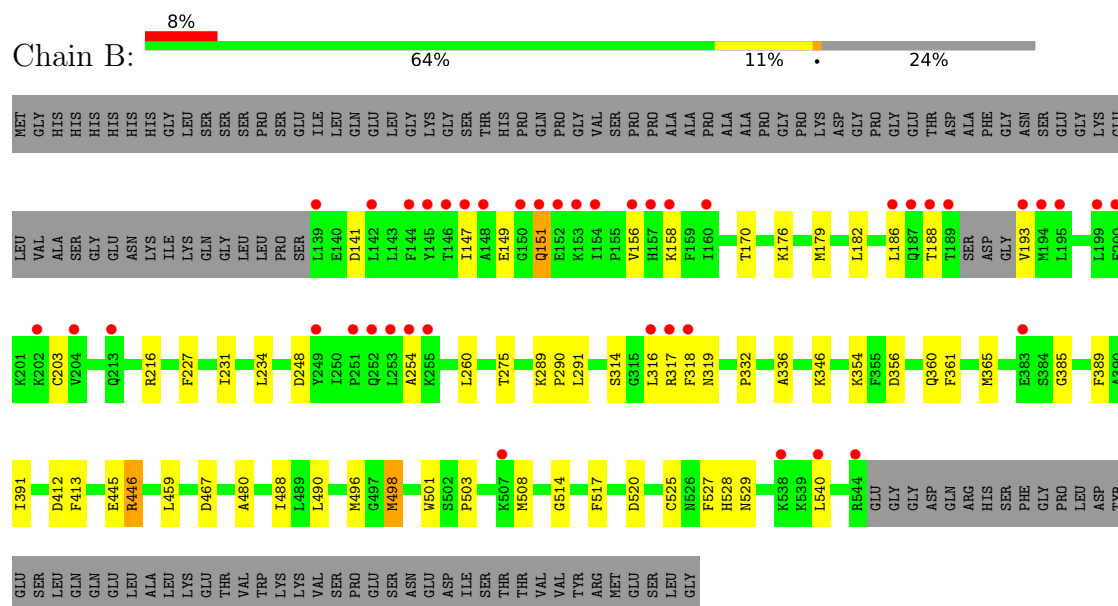
3 Residue-property plots

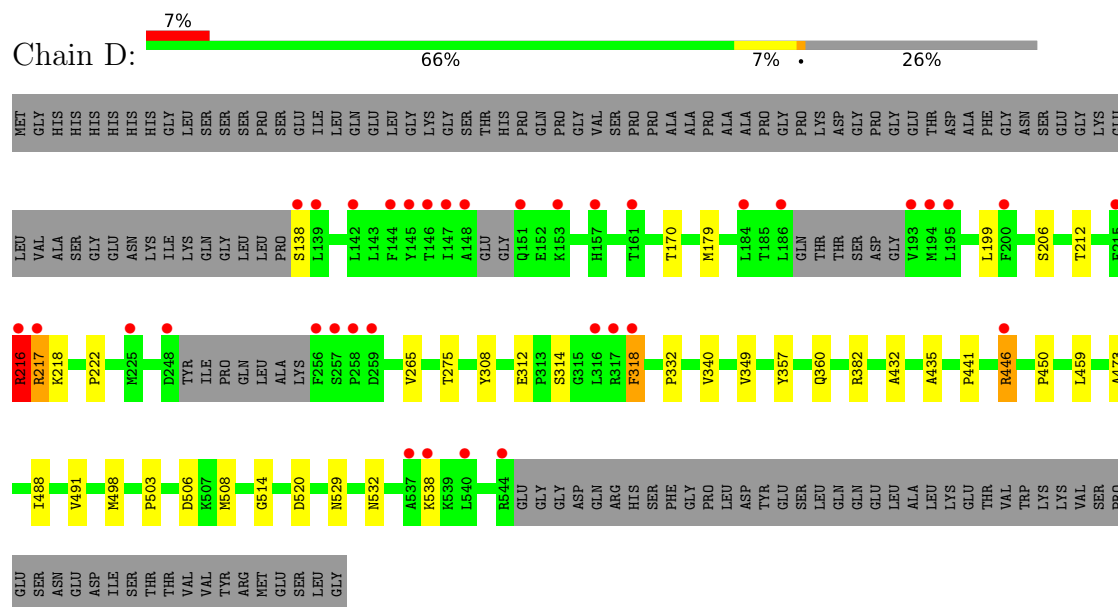
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Glutaminase kidney isoform, mitochondrial



- Molecule 1: Glutaminase kidney isoform, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.65Å 139.51Å 178.09Å 90.00° 93.49° 90.00°	Depositor
Resolution (Å)	109.99 – 2.39 109.99 – 2.39	Depositor EDS
% Data completeness (in resolution range)	92.9 (109.99-2.39) 92.9 (109.99-2.39)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.189 , 0.244 0.197 , 0.248	Depositor DCC
R_{free} test set	4490 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12864	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: V59

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	0.59	0/3208	1.06	5/4328 (0.1%)
1	B	0.59	0/3225	1.05	1/4352 (0.0%)
1	C	0.58	0/3142	1.06	2/4236 (0.0%)
1	D	0.59	0/3133	1.05	5/4223 (0.1%)
All	All	0.59	0/12708	1.06	13/17139 (0.1%)

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	A	0	1
1	B	0	1
1	D	0	3
All	All	0	5

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	318	PHE	CA-CB-CG	8.29	122.08	113.80
1	B	503	PRO	N-CA-C	7.86	120.28	110.70
1	A	503	PRO	N-CA-C	7.41	119.74	110.70
1	C	503	PRO	N-CA-C	7.17	119.45	110.70
1	D	503	PRO	N-CA-C	6.67	118.84	110.70
1	D	506	ASP	CA-CB-CG	6.58	119.18	112.60
1	A	275	THR	CB-CA-C	5.61	120.46	109.35
1	D	532	ASN	CB-CA-C	5.50	118.73	109.48
1	A	141	ASP	CA-CB-CG	5.27	117.87	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	GLU	CB-CA-C	-5.11	102.06	109.97
1	A	303	GLU	N-CA-C	-5.07	105.84	111.36
1	D	520	ASP	CA-CB-CG	5.04	117.64	112.60
1	D	275	THR	CB-CA-C	5.04	119.61	109.38

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	307	ARG	Sidechain
1	B	446	ARG	Sidechain
1	D	216	ARG	Sidechain
1	D	217	ARG	Sidechain
1	D	446	ARG	Sidechain

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	3138	0	3124	35	0
1	B	3155	0	3141	42	0
1	C	3076	0	3055	40	0
1	D	3067	0	3049	36	0
2	B	34	0	0	0	0
2	C	34	0	0	1	0
3	A	94	0	0	1	0
3	B	87	0	0	0	0
3	C	85	0	0	2	0
3	D	94	0	0	3	0
All	All	12864	0	12369	135	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (135) 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:D:265:VAL:HG22	1:D:498:MET:HE3	1.54	0.86
1:D:216:ARG:HB3	1:D:218:LYS:HG2	1.57	0.85
1:B:216:ARG:HG3	1:B:216:ARG:HH11	1.40	0.85
1:C:314:SER:HB2	1:C:318:PHE:HB3	1.59	0.85
1:B:317:ARG:HD2	1:D:318:PHE:HZ	1.47	0.80
1:A:248:ASP:HA	1:A:254:ALA:HB2	1.67	0.76
1:C:157:HIS:O	1:C:161:THR:HG22	1.90	0.70
1:A:234:LEU:HD22	1:A:520:ASP:HB3	1.74	0.69
1:B:216:ARG:HH11	1:B:216:ARG:CG	2.04	0.69
1:B:316:LEU:HD11	1:D:312:GLU:OE1	1.93	0.67
1:C:156:VAL:HG23	1:C:195:LEU:HD13	1.75	0.67
1:D:217:ARG:HE	1:D:222:PRO:HB2	1.61	0.66
1:D:314:SER:HB2	1:D:318:PHE:HB3	1.78	0.66
1:A:529:ASN:ND2	1:C:530:TYR:OH	2.28	0.66
1:B:318:PHE:HZ	1:D:318:PHE:CD1	2.15	0.65
1:A:138:SER:N	3:A:602:HOH:O	2.31	0.64
1:C:218:LYS:O	1:C:218:LYS:HD3	1.98	0.64
1:A:324:ASN:HA	1:C:317:ARG:HH12	1.64	0.62
1:B:227:PHE:CZ	1:B:231:ILE:HD11	2.35	0.62
1:C:398:LYS:NZ	3:C:701:HOH:O	2.32	0.62
1:B:182:LEU:HD23	1:B:203:CYS:SG	2.40	0.61
1:C:332:PRO:HD2	1:C:459:LEU:HD13	1.83	0.60
1:B:318:PHE:CZ	1:D:318:PHE:CD1	2.90	0.60
1:B:332:PRO:HD2	1:B:459:LEU:HD13	1.84	0.59
1:A:427:ALA:HB1	1:A:499:MET:HE2	1.84	0.58
1:A:227:PHE:CZ	1:A:496:MET:HE1	2.39	0.58
1:B:529:ASN:ND2	1:D:529:ASN:ND2	2.51	0.58
1:C:182:LEU:HD23	1:C:203:CYS:SG	2.43	0.58
1:B:529:ASN:CG	1:D:529:ASN:HD21	2.11	0.58
1:D:265:VAL:CG2	1:D:498:MET:HE3	2.30	0.56
1:B:488:ILE:HD12	1:B:514:GLY:HA3	1.88	0.56
1:B:291:LEU:HD22	1:B:365:MET:HE1	1.86	0.56
1:D:332:PRO:HD2	1:D:459:LEU:HD13	1.88	0.55
1:B:193:VAL:HG12	1:B:193:VAL:O	2.07	0.55
1:C:186:LEU:HD23	1:C:186:LEU:O	2.06	0.55
1:B:216:ARG:CG	1:B:216:ARG:NH1	2.69	0.54
1:A:201:LYS:HE3	1:A:205:GLN:HE21	1.73	0.54
1:C:318:PHE:CE1	1:C:321:LEU:HD12	2.41	0.54
1:A:182:LEU:HD23	1:A:203:CYS:SG	2.48	0.54
1:B:467:ASP:HB2	1:B:508:MET:HE2	1.90	0.54
1:B:248:ASP:HA	1:B:254:ALA:HB2	1.89	0.54
1:D:332:PRO:CD	1:D:459:LEU:HD13	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:VAL:HG22	1:C:436:ASN:HB2	1.90	0.53
1:B:529:ASN:CG	1:D:529:ASN:ND2	2.67	0.53
1:C:170:THR:HB	1:C:179:MET:HE2	1.90	0.53
1:C:291:LEU:HD22	1:C:365:MET:HE1	1.90	0.53
1:C:166:THR:HG21	1:C:214:ALA:HB1	1.91	0.52
1:C:153:LYS:HB3	1:C:194:MET:CE	2.40	0.52
1:A:525:CYS:HA	1:A:540:LEU:O	2.09	0.52
1:D:432:ALA:HB1	1:D:441:PRO:HG3	1.93	0.51
1:B:227:PHE:CZ	1:B:496:MET:HE1	2.46	0.51
1:A:507:LYS:CD	1:A:507:LYS:N	2.74	0.50
1:C:488:ILE:HD12	1:C:514:GLY:HA3	1.94	0.49
1:D:217:ARG:O	1:D:222:PRO:HB3	2.13	0.49
1:D:446:ARG:HH22	1:D:450:PRO:HG3	1.77	0.49
1:A:170:THR:O	1:A:179:MET:HG3	2.13	0.49
1:A:195:LEU:CD2	1:A:199:LEU:HD22	2.43	0.49
1:D:435:ALA:HB2	1:D:491:VAL:HG13	1.95	0.49
1:C:432:ALA:HB1	1:C:441:PRO:HG3	1.95	0.49
1:A:201:LYS:O	1:A:205:GLN:HG3	2.12	0.48
1:A:432:ALA:HB1	1:A:441:PRO:HG3	1.94	0.48
1:A:318:PHE:HE2	1:C:318:PHE:HB2	1.79	0.48
1:B:317:ARG:HB2	1:D:318:PHE:CE2	2.48	0.48
1:A:468:PHE:HD1	1:A:508:MET:HE3	1.77	0.48
1:B:317:ARG:HB2	1:D:318:PHE:CZ	2.48	0.48
1:D:473:ALA:HA	3:D:651:HOH:O	2.13	0.48
1:A:225:MET:HE2	1:A:225:MET:HA	1.95	0.48
1:A:507:LYS:CD	1:A:507:LYS:H	2.26	0.48
1:B:147:ILE:O	1:B:158:LYS:HE2	2.13	0.48
1:A:142:LEU:O	1:A:146:THR:HG23	2.13	0.48
1:B:498:MET:HE1	1:B:517:PHE:CE1	2.48	0.48
1:A:314:SER:HB2	1:A:318:PHE:HB2	1.95	0.47
1:A:148:ALA:O	1:A:151:GLN:HG2	2.14	0.47
1:B:317:ARG:NH1	1:D:318:PHE:CZ	2.77	0.47
1:B:319:ASN:HD22	1:B:467:ASP:CG	2.23	0.47
1:C:193:VAL:HG12	1:C:193:VAL:O	2.15	0.47
1:B:234:LEU:HD22	1:B:520:ASP:HB3	1.98	0.46
1:C:332:PRO:CD	1:C:459:LEU:HD13	2.46	0.46
1:D:216:ARG:HA	1:D:216:ARG:HD2	1.57	0.46
1:B:354:LYS:HB3	1:B:413:PHE:CZ	2.51	0.45
1:C:498:MET:HE1	1:C:517:PHE:CE1	2.51	0.45
1:D:216:ARG:C	1:D:218:LYS:N	2.71	0.45
1:D:308:TYR:HB3	1:D:340:VAL:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:GLN:NE2	1:C:311:LYS:HD2	2.32	0.45
1:B:289:LYS:N	1:B:290:PRO:HD2	2.31	0.45
1:C:200:PHE:O	1:C:204:VAL:HG22	2.16	0.45
1:A:200:PHE:O	1:A:204:VAL:HG22	2.17	0.45
1:C:318:PHE:CD1	1:C:321:LEU:HD12	2.52	0.45
1:C:227:PHE:CZ	1:C:496:MET:HE1	2.52	0.44
1:D:382:ARG:NH1	3:D:607:HOH:O	2.50	0.44
1:B:318:PHE:CZ	1:D:318:PHE:CE1	3.05	0.44
1:B:525:CYS:HA	1:B:540:LEU:O	2.18	0.44
1:C:389:PHE:CD1	1:C:411:LEU:HD13	2.52	0.44
1:A:293:TYR:HH	1:A:306:HIS:HE2	1.65	0.44
1:A:181:MET:O	1:A:185:THR:HG23	2.17	0.43
1:C:321:LEU:HB3	2:C:601:V59:N2	2.33	0.43
1:C:140:GLU:N	3:C:708:HOH:O	2.51	0.43
1:B:319:ASN:ND2	1:B:467:ASP:OD2	2.49	0.43
1:A:315:GLY:O	1:A:316:LEU:C	2.61	0.43
1:D:217:ARG:HE	1:D:217:ARG:HB3	1.61	0.43
1:B:356:ASP:O	1:B:360:GLN:HG2	2.18	0.43
1:B:260:LEU:HD13	1:B:501:TRP:HH2	1.83	0.43
1:A:479:PRO:HG3	1:C:530:TYR:CE1	2.54	0.43
1:B:527:PHE:O	1:B:528:HIS:C	2.62	0.43
1:D:217:ARG:NE	1:D:222:PRO:HB2	2.32	0.43
1:A:178:CYS:HA	1:A:203:CYS:O	2.19	0.42
1:C:260:LEU:HD13	1:C:501:TRP:HH2	1.84	0.42
1:B:314:SER:HB2	1:B:318:PHE:HB2	2.02	0.42
1:D:357:TYR:HA	1:D:360:GLN:HE21	1.84	0.42
1:B:170:THR:HB	1:B:179:MET:HE2	2.00	0.42
1:C:162:ALA:HB1	1:C:215:PHE:HE1	1.85	0.42
1:B:317:ARG:CD	1:D:318:PHE:HZ	2.25	0.42
1:C:495:VAL:HG12	1:C:496:MET:HE2	2.00	0.42
1:C:247:ALA:CB	1:C:484:VAL:HG22	2.49	0.42
1:C:379:GLN:O	1:C:382:ARG:HG2	2.20	0.41
1:D:212:THR:O	1:D:216:ARG:HB2	2.19	0.41
1:A:285:GLN:O	1:A:288:VAL:HG12	2.20	0.41
1:A:312:GLU:OE1	1:C:316:LEU:HD11	2.20	0.41
1:D:138:SER:N	3:D:609:HOH:O	2.53	0.41
1:D:170:THR:O	1:D:179:MET:HG3	2.20	0.41
1:A:142:LEU:HD23	1:A:142:LEU:HA	1.92	0.41
1:D:488:ILE:HD12	1:D:514:GLY:HA3	2.03	0.41
1:C:289:LYS:N	1:C:290:PRO:CD	2.84	0.41
1:C:175:LEU:O	1:C:179:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:SER:O	1:A:172:ASP:C	2.63	0.41
1:A:272:ARG:HH22	1:A:369:GLU:CD	2.29	0.41
1:B:346:LYS:HB3	1:B:354:LYS:HG2	2.02	0.41
1:B:385:GLY:O	1:B:389:PHE:HD2	2.03	0.41
1:C:281:PRO:HA	1:C:422:VAL:O	2.20	0.41
1:A:379:GLN:O	1:A:382:ARG:HG2	2.21	0.41
1:B:332:PRO:CD	1:B:459:LEU:HD13	2.49	0.41
1:C:171:SER:O	1:C:172:ASP:C	2.65	0.40
1:B:336:ALA:HA	1:B:391:ILE:HG21	2.03	0.40
1:B:480:ALA:HB2	1:B:490:LEU:HD12	2.02	0.40
1:D:308:TYR:HB3	1:D:340:VAL:HG11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	397/533 (74%)	388 (98%)	8 (2%)	1 (0%)	36	50
1	B	399/533 (75%)	383 (96%)	14 (4%)	2 (0%)	24	37
1	C	385/533 (72%)	372 (97%)	13 (3%)	0	100	100
1	D	384/533 (72%)	369 (96%)	15 (4%)	0	100	100
All	All	1565/2132 (73%)	1512 (97%)	50 (3%)	3 (0%)	43	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	537	ALA
1	B	149	GLU
1	B	151	GLN

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	348/456 (76%)	340 (98%)	8 (2%)	44	66
1	B	350/456 (77%)	338 (97%)	12 (3%)	32	54
1	C	342/456 (75%)	330 (96%)	12 (4%)	32	53
1	D	341/456 (75%)	334 (98%)	7 (2%)	47	69
All	All	1381/1824 (76%)	1342 (97%)	39 (3%)	38	60

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	GLU
1	A	199	LEU
1	A	245	LYS
1	A	303	GLU
1	A	317	ARG
1	A	399	LYS
1	A	507	LYS
1	A	540	LEU
1	B	141	ASP
1	B	151	GLN
1	B	156	VAL
1	B	176	LYS
1	B	186	LEU
1	B	188	THR
1	B	275	THR
1	B	361	PHE
1	B	412	ASP
1	B	445	GLU
1	B	446	ARG
1	B	498	MET
1	C	156	VAL
1	C	161	THR
1	C	176	LYS
1	C	188	THR

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Mol	Chain	Res	Type
1	C	206	SER
1	C	268	VAL
1	C	275	THR
1	C	317	ARG
1	C	318	PHE
1	C	320	LYS
1	C	361	PHE
1	C	538	LYS
1	D	199	LEU
1	D	206	SER
1	D	216	ARG
1	D	318	PHE
1	D	349	VAL
1	D	508	MET
1	D	538	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	HIS
1	A	205	GLN
1	A	330	HIS
1	A	471	GLN
1	A	516	HIS
1	A	529	ASN
1	B	230	HIS
1	B	335	ASN
1	B	516	HIS
1	C	151	GLN
1	C	230	HIS
1	C	347	GLN
1	C	516	HIS
1	C	529	ASN
1	D	330	HIS
1	D	347	GLN
1	D	360	GLN
1	D	388	ASN
1	D	436	ASN
1	D	529	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	V59	B	601	-	38,38,38	1.56	3 (7%)	43,51,51	1.76	6 (13%)
2	V59	C	601	-	38,38,38	1.57	3 (7%)	43,51,51	1.50	7 (16%)

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	V59	B	601	-	-	4/20/29/29	0/5/5/5
2	V59	C	601	-	-	4/20/29/29	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	V59	C2-S1	6.32	1.84	1.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	V59	C3-S1	6.20	1.84	1.73
2	B	601	V59	C3-S1	6.07	1.84	1.73
2	B	601	V59	C2-S1	6.01	1.84	1.73
2	B	601	V59	C2-N2	2.06	1.34	1.31
2	C	601	V59	C2-N2	2.00	1.34	1.31

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	V59	C1-N1-C2	6.37	134.58	123.69
2	B	601	V59	C16-O2-C15	5.97	132.43	118.78
2	C	601	V59	C1-N1-C2	5.75	133.51	123.69
2	C	601	V59	C11-N5-C7	3.83	128.23	123.58
2	B	601	V59	C11-N5-C7	3.02	127.24	123.58
2	C	601	V59	C5-C4-C11	-2.99	98.04	103.33
2	B	601	V59	C5-C4-C11	-2.85	98.29	103.33
2	C	601	V59	C10-N6-N7	2.63	120.92	118.91
2	C	601	V59	C16-O2-C15	2.48	124.44	118.78
2	B	601	V59	C4-N4-C3	-2.40	120.27	124.48
2	C	601	V59	C4-N4-C3	-2.36	120.34	124.48
2	B	601	V59	C8-C7-N7	-2.35	120.40	123.84
2	C	601	V59	C8-C7-N7	-2.25	120.54	123.84

There are no chirality outliers.

All (8) torsion outliers are listed below:

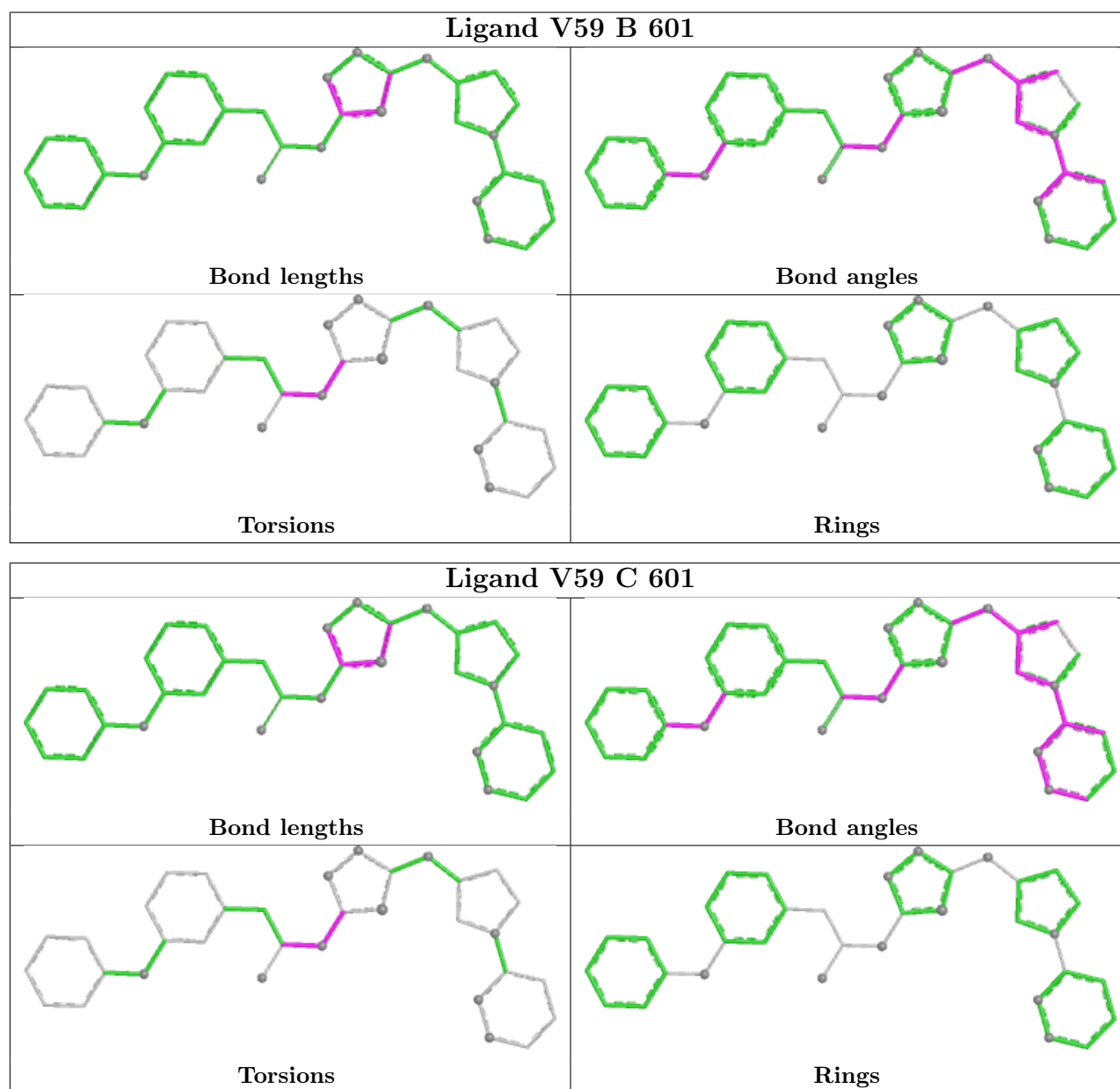
Mol	Chain	Res	Type	Atoms
2	B	601	V59	O1-C1-N1-C2
2	B	601	V59	C12-C1-N1-C2
2	C	601	V59	O1-C1-N1-C2
2	B	601	V59	S1-C2-N1-C1
2	C	601	V59	C12-C1-N1-C2
2	B	601	V59	N2-C2-N1-C1
2	C	601	V59	S1-C2-N1-C1
2	C	601	V59	N2-C2-N1-C1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	V59	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	401/533 (75%)	0.49	38 (9%) 14 11	26, 40, 86, 124	0
1	B	403/533 (75%)	0.52	42 (10%) 11 9	25, 39, 88, 119	0
1	C	393/533 (73%)	0.67	42 (10%) 11 8	28, 43, 88, 113	0
1	D	392/533 (73%)	0.52	35 (8%) 15 12	26, 41, 83, 128	0
All	All	1589/2132 (74%)	0.55	157 (9%) 13 9	25, 41, 86, 128	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	193	VAL	8.8
1	C	318	PHE	7.4
1	D	318	PHE	7.0
1	A	193	VAL	6.6
1	D	256	PHE	6.2
1	D	258	PRO	5.8
1	B	193	VAL	5.8
1	C	193	VAL	5.6
1	D	217	ARG	4.9
1	C	189	THR	4.8
1	A	253	LEU	4.7
1	A	186	LEU	4.7
1	C	144	PHE	4.7
1	C	317	ARG	4.6
1	B	139	LEU	4.6
1	C	195	LEU	4.6
1	C	202	LYS	4.5
1	A	249	TYR	4.5
1	B	145	TYR	4.4
1	D	316	LEU	4.4
1	C	538	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	538	LYS	4.3
1	D	186	LEU	4.2
1	A	316	LEU	4.2
1	C	200	PHE	4.0
1	B	544	ARG	4.0
1	B	254	ALA	4.0
1	C	256	PHE	4.0
1	B	316	LEU	3.9
1	B	142	LEU	3.8
1	D	446	ARG	3.8
1	C	316	LEU	3.8
1	B	318	PHE	3.7
1	C	148	ALA	3.7
1	B	200	PHE	3.6
1	B	540	LEU	3.6
1	D	148	ALA	3.6
1	A	318	PHE	3.6
1	C	186	LEU	3.5
1	A	142	LEU	3.5
1	A	540	LEU	3.5
1	B	317	ARG	3.5
1	D	216	ARG	3.4
1	B	153	LYS	3.4
1	C	145	TYR	3.4
1	A	250	ILE	3.3
1	A	317	ARG	3.3
1	C	153	LYS	3.3
1	C	540	LEU	3.3
1	C	142	LEU	3.2
1	B	147	ILE	3.2
1	B	252	GLN	3.2
1	B	144	PHE	3.2
1	D	215	PHE	3.2
1	B	538	LYS	3.2
1	B	150	GLY	3.2
1	A	194	MET	3.2
1	C	544	ARG	3.1
1	D	225	MET	3.2
1	C	157	HIS	3.1
1	B	148	ALA	3.1
1	C	147	ILE	3.1
1	C	188	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	537	ALA	3.1
1	D	195	LEU	3.0
1	A	252	GLN	3.0
1	D	184	LEU	3.0
1	B	154	ILE	3.0
1	D	151	GLN	3.0
1	A	145	TYR	2.9
1	A	251	PRO	2.9
1	C	199	LEU	2.9
1	D	145	TYR	2.9
1	B	157	HIS	2.9
1	A	544	ARG	2.9
1	B	195	LEU	2.9
1	A	225	MET	2.9
1	A	254	ALA	2.9
1	D	153	LYS	2.8
1	B	249	TYR	2.8
1	B	151	GLN	2.8
1	A	195	LEU	2.8
1	B	189	THR	2.8
1	D	147	ILE	2.7
1	B	156	VAL	2.7
1	C	151	GLN	2.7
1	C	185	THR	2.7
1	A	153	LYS	2.7
1	A	256	PHE	2.7
1	A	152	GLU	2.7
1	D	142	LEU	2.7
1	A	507	LYS	2.7
1	C	204	VAL	2.6
1	D	138	SER	2.6
1	C	194	MET	2.6
1	B	186	LEU	2.6
1	B	204	VAL	2.6
1	C	140	GLU	2.6
1	C	152	GLU	2.6
1	C	248	ASP	2.6
1	A	184	LEU	2.5
1	C	143	LEU	2.5
1	B	188	THR	2.5
1	C	156	VAL	2.5
1	C	467	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	146	THR	2.5
1	B	152	GLU	2.5
1	B	199	LEU	2.5
1	D	257	SER	2.4
1	C	180	ASP	2.4
1	A	150	GLY	2.4
1	D	144	PHE	2.4
1	B	507	LYS	2.4
1	C	225	MET	2.4
1	C	184	LEU	2.4
1	B	187	GLN	2.4
1	C	201	LYS	2.4
1	B	255	LYS	2.3
1	A	156	VAL	2.3
1	D	200	PHE	2.3
1	C	258	PRO	2.3
1	D	157	HIS	2.3
1	A	139	LEU	2.3
1	A	202	LYS	2.3
1	C	507	LYS	2.3
1	A	148	ALA	2.3
1	A	185	THR	2.3
1	D	146	THR	2.3
1	C	209	VAL	2.3
1	D	259	ASP	2.2
1	D	194	MET	2.2
1	B	202	LYS	2.2
1	D	161	THR	2.2
1	C	154	ILE	2.2
1	D	317	ARG	2.2
1	B	146	THR	2.2
1	A	216	ARG	2.2
1	D	540	LEU	2.2
1	D	544	ARG	2.2
1	A	196	ASP	2.2
1	A	529	ASN	2.2
1	B	383	GLU	2.2
1	B	253	LEU	2.1
1	D	139	LEU	2.1
1	D	248	ASP	2.1
1	A	537	ALA	2.1
1	B	160	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	320	LYS	2.1
1	B	213	GLN	2.1
1	A	538	LYS	2.1
1	A	536	PHE	2.1
1	A	157	HIS	2.1
1	B	251	PRO	2.1
1	A	138	SER	2.0
1	B	194	MET	2.0
1	B	158	LYS	2.0
1	C	158	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

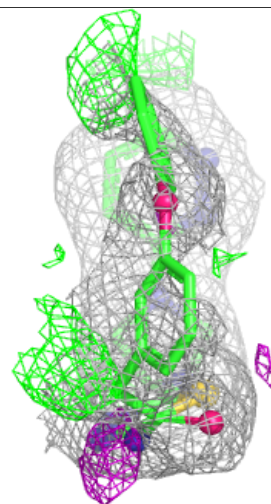
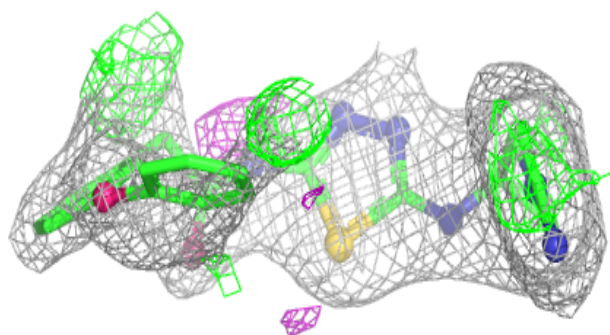
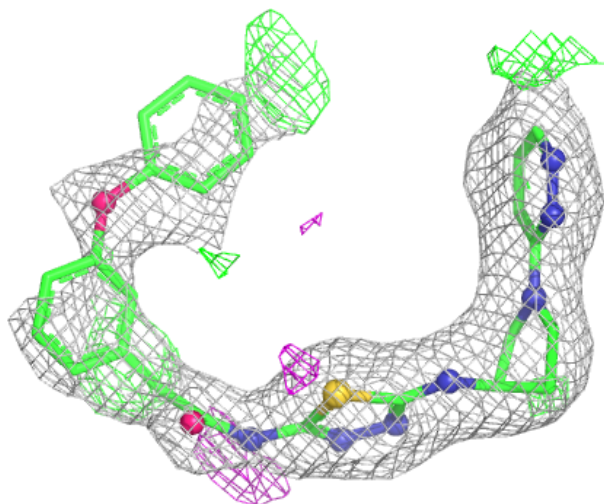
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	V59	B	601	34/34	0.90	0.18	29,54,107,119	0
2	V59	C	601	34/34	0.93	0.16	29,48,117,124	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.

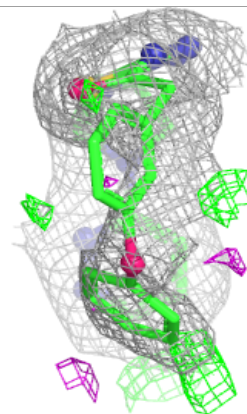
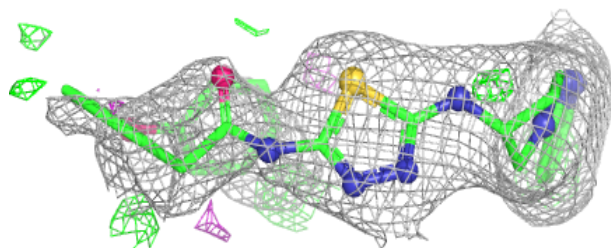
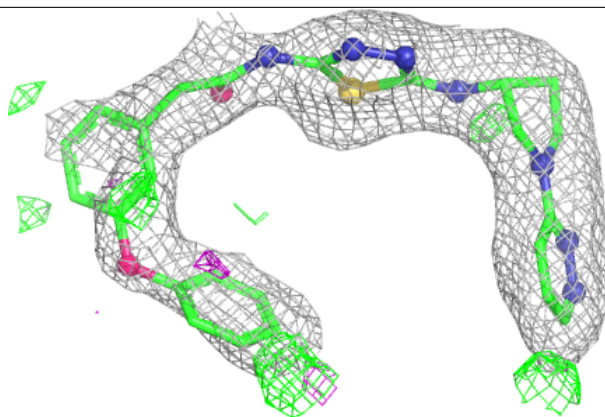
Electron density around V59 B 601:

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



Electron density around V59 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.