



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2020 – 11:11 AM EDT

PDB ID : 6UL9  
Title : Crystal structure of human GAC in complex with inhibitor UPGL00023  
Authors : Huang, Q.Q.; Cerione, R.A.  
Deposited on : 2019-10-07  
Resolution : 2.50 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](mailto: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.

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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 : 2.14.6  
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) : 2.14.6

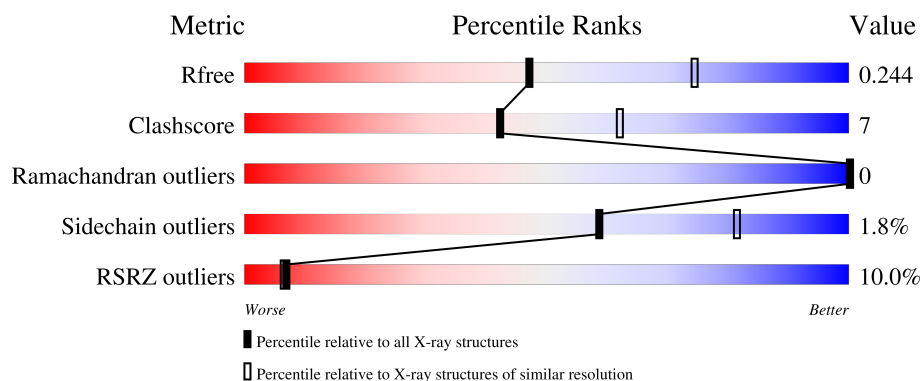
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	527	<div> <div>7%</div> <div>63% 12% 24%</div> </div>
1	B	527	<div> <div>7%</div> <div>63% 13% 22%</div> </div>
1	C	527	<div> <div>9%</div> <div>67% 10% 22%</div> </div>
1	D	527	<div> <div>7%</div> <div>66% 11% 22%</div> </div>

## 2 Entry composition [i](#)

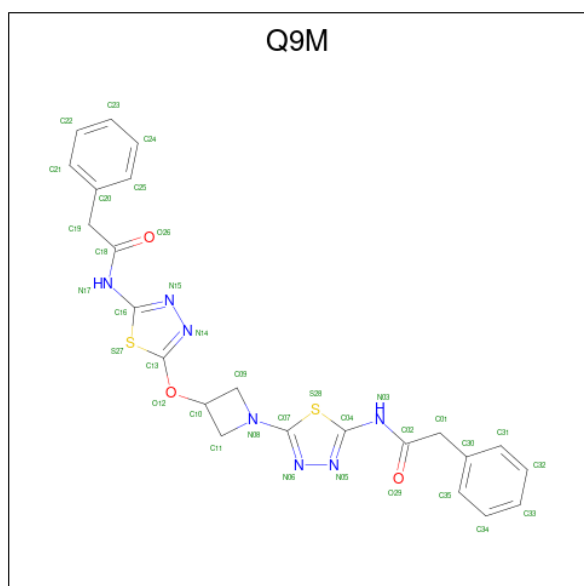
There are 3 unique types of molecules in this entry. The entry contains 13389 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	402	Total	C	N	O	S	1	0	0
			3135	1996	530	581	28			
1	B	409	Total	C	N	O	S	1	0	0
			3192	2036	539	589	28			
1	C	410	Total	C	N	O	S	1	0	0
			3196	2038	540	590	28			
1	D	409	Total	C	N	O	S	1	0	0
			3192	2036	539	589	28			

- Molecule 2 is 2-phenyl-N-{5-[(1-{5-[(phenylacetyl)amino]-1,3,4-thiadiazol-2-yl}azetidin-3-yl)oxy]-1,3,4-thiadiazol-2-yl}acetamide (three-letter code: Q9M) (formula: C<sub>23</sub>H<sub>21</sub>N<sub>7</sub>O<sub>3</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			35	23	7	3	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	S	0	0
			35	23	7	3	2		

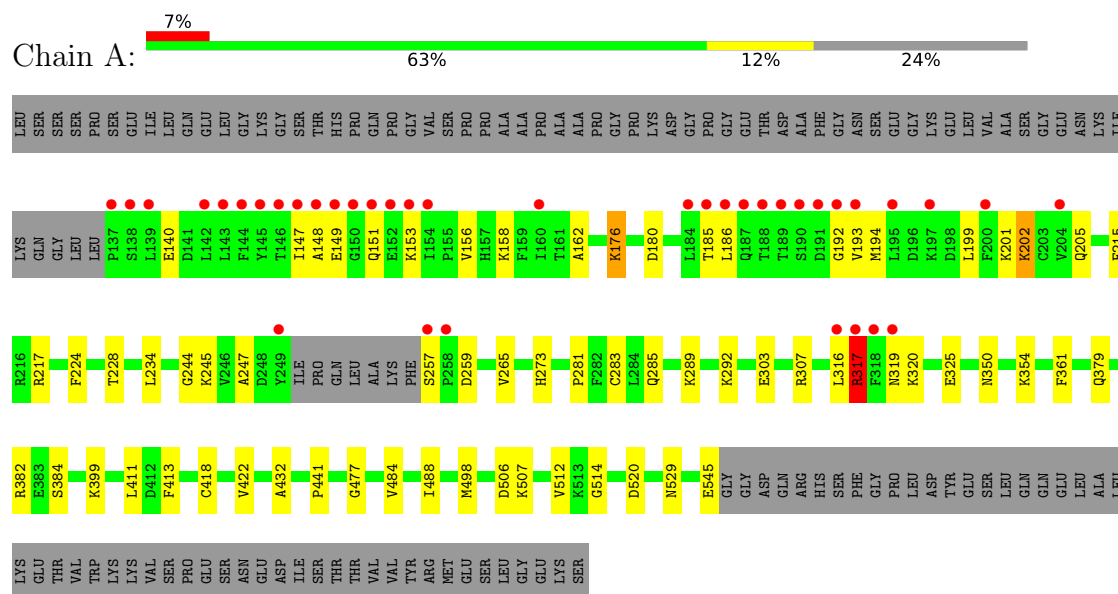
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	160	Total	O	0	0
			160	160		
3	B	156	Total	O	0	0
			156	156		
3	C	133	Total	O	0	0
			133	133		
3	D	155	Total	O	0	0
			155	155		

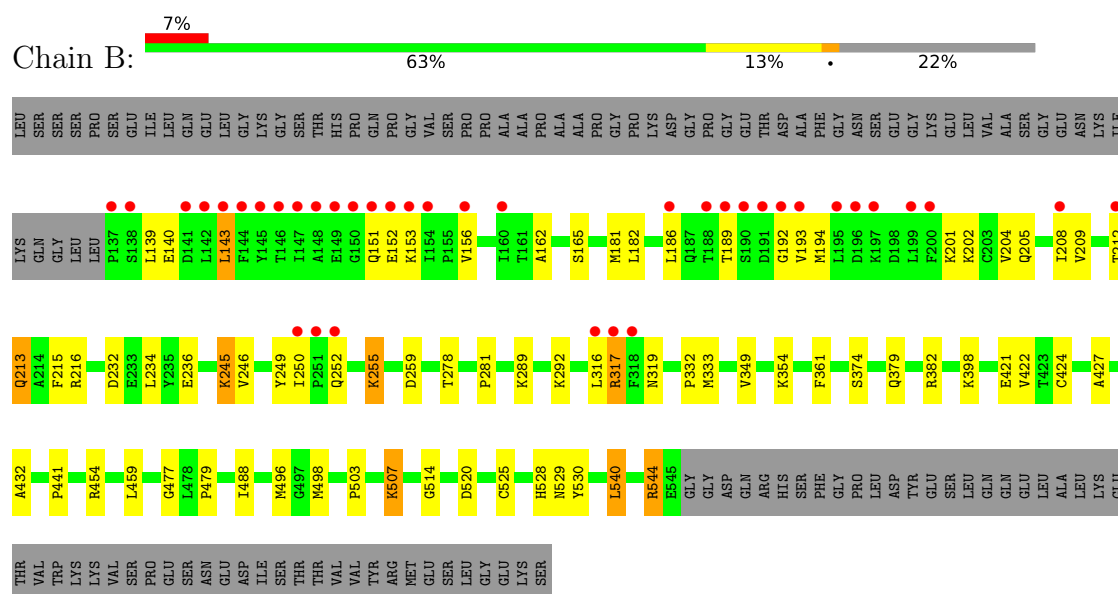
### 3 Residue-property plots

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.

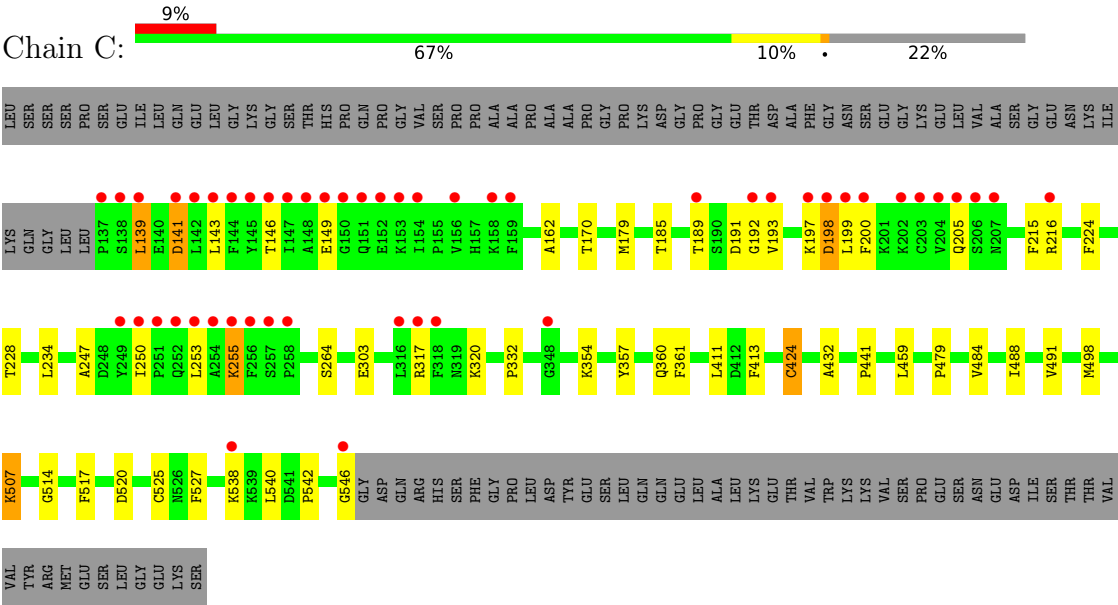
- Molecule 1: Glutaminase kidney isoform, mitochondrial



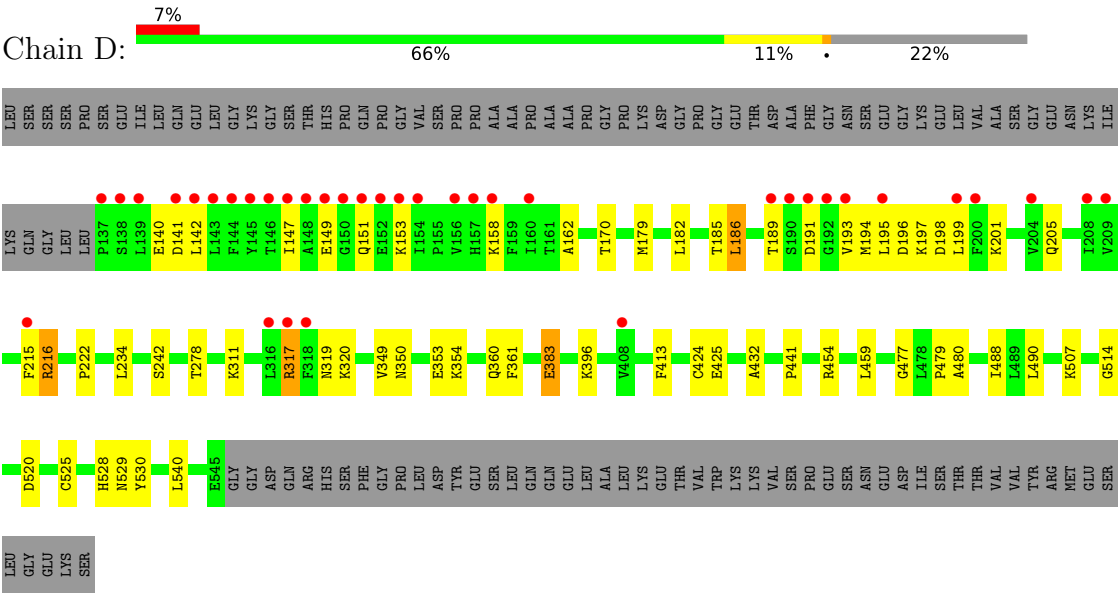
- Molecule 1: Glutaminase kidney isoform, mitochondrial



- Molecule 1: Glutaminase kidney isoform, mitochondrial



● Molecule 1: Glutaminase kidney isoform, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.88Å 138.24Å 176.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.94 – 2.50 48.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.94-2.50) 99.3 (48.94-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.20	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.10 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.192 , 0.244 0.192 , 0.244	Depositor DCC
$R_{free}$ test set	1999 reflections (2.42%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13389	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	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 52.00 % 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 5.1778e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: Q9M

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	0.50	2/3204 (0.1%)	0.70	7/4323 (0.2%)
1	B	0.46	0/3264	0.64	2/4406 (0.0%)
1	C	0.47	1/3268 (0.0%)	0.69	5/4411 (0.1%)
1	D	0.45	0/3264	0.63	2/4406 (0.0%)
All	All	0.47	3/13000 (0.0%)	0.66	16/17546 (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	C	0	1
1	D	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	424	CYS	CB-SG	-6.33	1.71	1.82
1	A	320	LYS	CD-CE	5.77	1.65	1.51
1	A	283	CYS	CB-SG	-5.62	1.72	1.81

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	538	LYS	CD-CE-NZ	-11.52	85.20	111.70
1	D	383	GLU	CA-CB-CG	7.25	129.36	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	LYS	CA-CB-CG	-7.17	97.63	113.40
1	C	198	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	A	399	LYS	CD-CE-NZ	5.99	125.47	111.70
1	B	540	LEU	CA-CB-CG	5.94	128.97	115.30
1	A	202	LYS	CA-CB-CG	5.84	126.24	113.40
1	D	142	LEU	CA-CB-CG	-5.59	102.43	115.30
1	A	185	THR	C-N-CA	-5.51	107.92	121.70
1	C	538	LYS	CB-CG-CD	-5.51	97.28	111.60
1	C	198	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	176	LYS	CB-CG-CD	5.44	125.76	111.60
1	C	149	GLU	CA-CB-CG	5.22	124.88	113.40
1	B	143	LEU	CB-CG-CD2	-5.19	102.17	111.00
1	A	325	GLU	N-CA-CB	-5.18	101.28	110.60
1	A	320	LYS	CA-CB-CG	5.17	124.77	113.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	317	ARG	Peptide
1	B	317	ARG	Peptide
1	C	317	ARG	Peptide
1	D	317	ARG	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	3135	0	3106	39	1
1	B	3192	0	3171	62	1
1	C	3196	0	3174	34	1
1	D	3192	0	3171	47	0
2	B	35	0	0	2	0
2	D	35	0	0	1	0
3	A	160	0	0	3	0
3	B	156	0	0	2	1
3	C	133	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	155	0	0	4	0
All	All	13389	0	12622	176	2

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 (176) 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:B:139:LEU:O	1:B:143:LEU:HD13	1.28	1.32
1:A:186:LEU:HD22	1:A:193:VAL:HG21	1.35	1.07
1:C:185:THR:O	1:C:189:THR:OG1	1.87	0.91
1:B:139:LEU:O	1:B:143:LEU:CD1	2.21	0.87
1:D:350:ASN:ND2	1:D:353:GLU:OE2	2.10	0.85
1:B:143:LEU:HD21	1:B:212:THR:OG1	1.84	0.78
1:D:141:ASP:CG	1:D:197:LYS:HE2	2.04	0.77
1:A:147:ILE:O	1:A:158:LYS:NZ	2.18	0.76
1:A:186:LEU:HD22	1:A:193:VAL:CG2	2.15	0.75
1:B:143:LEU:HD22	1:B:208:ILE:HD11	1.67	0.75
1:A:234:LEU:HD22	1:A:520:ASP:HB3	1.69	0.75
1:D:151:GLN:HE22	1:D:194:MET:HE3	1.52	0.74
1:D:317:ARG:HD2	1:D:320:LYS:HE3	1.70	0.73
1:B:153:LYS:HB2	1:B:194:MET:HE2	1.70	0.72
1:B:234:LEU:HD22	1:B:520:ASP:HB3	1.72	0.72
1:B:189:THR:HG22	1:C:255:LYS:HD3	1.72	0.71
1:D:151:GLN:HE22	1:D:194:MET:CE	2.03	0.71
1:A:186:LEU:CD2	1:A:193:VAL:HG21	2.19	0.69
1:C:234:LEU:HD22	1:C:520:ASP:HB3	1.73	0.69
1:A:319:ASN:ND2	3:A:603:HOH:O	2.26	0.69
1:B:529:ASN:OD1	1:D:529:ASN:ND2	2.25	0.68
1:C:146:THR:HG21	1:C:216:ARG:NH1	2.08	0.68
1:B:151:GLN:HG3	1:B:152:GLU:N	2.10	0.67
1:D:234:LEU:HD22	1:D:520:ASP:HB3	1.76	0.66
1:B:162:ALA:O	1:B:165:SER:HB3	1.95	0.66
1:D:182:LEU:O	1:D:186:LEU:HD12	1.95	0.66
1:C:498:MET:HE1	1:C:517:PHE:CE1	2.31	0.66
1:C:146:THR:HG21	1:C:216:ARG:HH12	1.61	0.65
1:B:349:VAL:O	1:B:354:LYS:HE3	1.98	0.63
1:D:317:ARG:HA	1:D:319:ASN:OD1	1.99	0.62
1:A:176:LYS:HD3	1:A:180:ASP:OD2	2.03	0.58
1:A:199:LEU:O	1:A:202:LYS:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:LYS:HD2	1:B:246:VAL:O	2.04	0.58
1:C:488:ILE:HD12	1:C:514:GLY:HA3	1.87	0.57
1:A:217:ARG:NH1	1:A:545:GLU:OE2	2.35	0.56
1:B:181:MET:HE2	1:B:202:LYS:HG2	1.88	0.56
1:D:195:LEU:HD23	1:D:199:LEU:HG	1.88	0.55
1:D:396:LYS:NZ	3:D:707:HOH:O	2.40	0.55
1:B:201:LYS:O	1:B:205:GLN:HB3	2.07	0.55
1:D:153:LYS:NZ	3:D:706:HOH:O	2.36	0.54
1:C:498:MET:HE1	1:C:517:PHE:HE1	1.72	0.54
1:B:151:GLN:HG3	1:B:152:GLU:H	1.72	0.54
1:A:162:ALA:HB1	1:A:215:PHE:HE1	1.73	0.54
1:B:530:TYR:CE1	1:D:479:PRO:HG3	2.43	0.54
1:A:477:GLY:O	1:A:529:ASN:HB2	2.08	0.53
1:B:232:ASP:O	1:B:236:GLU:HG2	2.08	0.53
1:B:422:VAL:HG21	1:B:427:ALA:HB2	1.91	0.53
1:B:525:CYS:HA	1:B:540:LEU:O	2.09	0.53
1:B:252:GLN:O	1:B:255:LYS:HG2	2.08	0.53
1:B:528:HIS:CD2	1:D:454:ARG:HD2	2.44	0.53
1:A:488:ILE:HD12	1:A:514:GLY:HA3	1.91	0.53
1:C:507:LYS:HE2	1:C:507:LYS:H	1.74	0.53
1:D:147:ILE:O	1:D:158:LYS:HE2	2.08	0.52
1:D:216:ARG:HA	1:D:216:ARG:HE	1.74	0.52
1:A:285:GLN:HA	1:A:418:CYS:HB3	1.91	0.52
1:B:162:ALA:HB1	1:B:215:PHE:HE1	1.74	0.52
1:B:432:ALA:HB1	1:B:441:PRO:HG2	1.91	0.52
1:B:181:MET:HE1	1:B:202:LYS:HE2	1.92	0.52
1:B:319:ASN:O	3:B:702:HOH:O	2.18	0.51
1:B:477:GLY:O	1:B:529:ASN:HB2	2.10	0.51
1:C:141:ASP:OD2	1:C:197:LYS:HD2	2.10	0.51
1:D:141:ASP:OD1	1:D:197:LYS:HE2	2.10	0.51
1:B:398:LYS:NZ	3:B:705:HOH:O	2.33	0.51
1:D:195:LEU:CD2	1:D:199:LEU:HG	2.39	0.50
1:B:143:LEU:N	1:B:143:LEU:HD12	2.26	0.50
1:B:479:PRO:HG3	1:D:530:TYR:CE1	2.46	0.50
1:A:244:GLY:C	1:A:245:LYS:HG2	2.32	0.50
1:D:349:VAL:O	1:D:354:LYS:HE3	2.09	0.50
1:A:316:LEU:HD21	3:A:720:HOH:O	2.11	0.50
1:B:316:LEU:O	1:B:319:ASN:ND2	2.44	0.50
1:A:303:GLU:CD	1:A:303:GLU:H	2.15	0.50
1:B:488:ILE:HD12	1:B:514:GLY:HA3	1.93	0.49
1:D:196:ASP:OD1	1:D:198:ASP:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:VAL:HG22	1:A:498:MET:HG2	1.95	0.49
1:D:185:THR:O	1:D:189:THR:HB	2.13	0.49
1:D:201:LYS:O	1:D:205:GLN:HB2	2.13	0.48
1:D:153:LYS:HB2	1:D:194:MET:HE1	1.93	0.48
1:A:247:ALA:HB2	1:A:484:VAL:HG22	1.94	0.48
1:A:317:ARG:HA	1:A:319:ASN:OD1	2.12	0.48
1:A:384:SER:OG	3:A:601:HOH:O	2.20	0.48
1:D:162:ALA:HB1	1:D:215:PHE:HE1	1.79	0.48
1:A:257:SER:OG	1:A:259:ASP:OD2	2.32	0.48
1:B:204:VAL:HG23	1:B:208:ILE:HD13	1.96	0.48
1:D:477:GLY:O	1:D:529:ASN:HB2	2.14	0.47
1:A:176:LYS:HG2	1:A:176:LYS:O	1.88	0.47
1:A:156:VAL:HG11	1:A:186:LEU:HD11	1.96	0.47
1:D:432:ALA:HB1	1:D:441:PRO:HG2	1.95	0.47
1:B:245:LYS:HB3	1:B:245:LYS:HE3	1.63	0.47
1:D:425:GLU:OE2	3:D:701:HOH:O	2.20	0.47
1:A:506:ASP:HB3	1:A:512:VAL:HG22	1.97	0.47
1:C:189:THR:HA	1:C:191:ASP:OD1	2.14	0.47
1:C:162:ALA:HB1	1:C:215:PHE:HE1	1.80	0.47
1:D:216:ARG:HA	1:D:216:ARG:NE	2.30	0.47
1:B:316:LEU:HA	1:B:316:LEU:HD23	1.68	0.46
1:B:156:VAL:HG21	1:B:186:LEU:HD21	1.97	0.46
1:C:357:TYR:O	1:C:360:GLN:HG3	2.16	0.46
1:B:153:LYS:CB	1:B:194:MET:HE2	2.41	0.46
1:C:479:PRO:HD2	1:C:491:VAL:O	2.16	0.46
1:C:332:PRO:HD2	1:C:459:LEU:HD13	1.97	0.46
1:A:140:GLU:OE1	1:A:205:GLN:HG2	2.16	0.46
1:B:374:SER:HB2	1:B:421:GLU:OE2	2.16	0.45
1:D:140:GLU:N	1:D:140:GLU:OE1	2.36	0.45
1:A:192:GLY:HA3	1:A:193:VAL:HA	1.58	0.45
1:B:496:MET:SD	1:B:498:MET:HE2	2.57	0.45
2:B:601:Q9M:O29	2:B:601:Q9M:N05	2.48	0.45
1:C:192:GLY:HA3	1:C:193:VAL:HA	1.53	0.45
1:C:354:LYS:HB3	1:C:413:PHE:CZ	2.52	0.45
1:B:140:GLU:N	1:B:140:GLU:OE1	2.40	0.45
1:B:289:LYS:HA	1:B:292:LYS:HE2	1.97	0.45
1:A:379:GLN:O	1:A:382:ARG:HG2	2.16	0.45
1:D:193:VAL:O	1:D:193:VAL:HG23	2.16	0.45
1:B:454:ARG:HD2	1:D:528:HIS:CD2	2.52	0.45
1:C:507:LYS:H	1:C:507:LYS:CE	2.30	0.45
1:B:507:LYS:H	1:B:507:LYS:HE2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:432:ALA:HB1	1:C:441:PRO:HG2	1.98	0.44
1:D:195:LEU:HD23	1:D:199:LEU:CG	2.47	0.44
1:D:222:PRO:HG3	3:D:745:HOH:O	2.18	0.44
2:D:601:Q9M:O26	2:D:601:Q9M:C25	2.64	0.44
1:B:192:GLY:HA3	1:B:193:VAL:HA	1.63	0.44
1:C:247:ALA:HB2	1:C:484:VAL:HG22	1.99	0.44
1:A:148:ALA:O	1:A:149:GLU:HB2	2.17	0.44
1:C:143:LEU:HD23	1:C:200:PHE:HZ	1.82	0.44
1:C:224:PHE:O	1:C:228:THR:HG23	2.18	0.44
1:C:303:GLU:CD	1:C:303:GLU:H	2.21	0.44
1:B:281:PRO:HA	1:B:422:VAL:O	2.18	0.43
1:D:149:GLU:HG3	1:D:149:GLU:O	2.18	0.43
1:A:289:LYS:HA	1:A:292:LYS:HE2	1.99	0.43
1:B:246:VAL:HG22	1:B:503:PRO:HB2	2.00	0.43
1:B:317:ARG:HA	1:B:319:ASN:OD1	2.18	0.43
1:B:544:ARG:HD3	1:B:544:ARG:HA	1.52	0.43
1:D:488:ILE:HD12	1:D:514:GLY:HA3	1.99	0.43
1:D:480:ALA:HB2	1:D:490:LEU:HD12	2.00	0.43
1:B:317:ARG:HE	2:B:601:Q9M:C22	2.32	0.43
1:C:527:PHE:CZ	1:C:542:PRO:HG2	2.54	0.43
1:D:317:ARG:HD2	1:D:320:LYS:CE	2.45	0.42
1:A:350:ASN:N	1:A:350:ASN:OD1	2.48	0.42
1:C:255:LYS:HE3	1:C:255:LYS:HB3	1.82	0.42
1:C:546:GLY:HA2	3:C:635:HOH:O	2.19	0.42
1:B:249:TYR:CD1	1:B:250:ILE:HG23	2.54	0.42
1:D:278:THR:HA	1:D:424:CYS:HB2	2.01	0.42
1:D:525:CYS:HA	1:D:540:LEU:O	2.18	0.42
1:B:278:THR:HA	1:B:424:CYS:HB2	2.01	0.42
1:C:250:ILE:HG13	1:C:253:LEU:HD12	2.01	0.42
1:A:354:LYS:HB3	1:A:413:PHE:CZ	2.54	0.42
1:C:170:THR:O	1:C:179:MET:HG3	2.20	0.42
1:A:411:LEU:HD23	1:A:411:LEU:HA	1.86	0.42
1:B:507:LYS:HB2	1:B:507:LYS:HE2	1.78	0.42
1:A:148:ALA:O	1:A:151:GLN:HB3	2.20	0.41
1:B:209:VAL:O	1:B:213:GLN:HB2	2.20	0.41
1:B:528:HIS:CG	1:D:454:ARG:HD2	2.54	0.41
1:D:354:LYS:HB3	1:D:413:PHE:CZ	2.55	0.41
1:A:224:PHE:O	1:A:228:THR:HG23	2.20	0.41
1:D:191:ASP:OD1	1:D:191:ASP:N	2.42	0.41
1:B:216:ARG:HA	1:B:216:ARG:HD2	1.65	0.41
1:B:379:GLN:O	1:B:382:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:ARG:HD2	1:D:528:HIS:CG	2.54	0.41
1:B:332:PRO:HB2	1:B:333:MET:HE3	2.02	0.41
1:C:264:SER:OG	1:C:424:CYS:HB3	2.20	0.41
1:A:228:THR:HB	1:A:273:HIS:CD2	2.56	0.41
1:A:153:LYS:HB3	1:A:194:MET:HB3	2.02	0.41
1:D:151:GLN:HE22	1:D:194:MET:HE1	1.83	0.41
1:A:281:PRO:HA	1:A:422:VAL:O	2.20	0.41
1:B:332:PRO:HD2	1:B:459:LEU:HD13	2.03	0.41
1:B:507:LYS:CE	1:B:507:LYS:H	2.34	0.41
1:C:139:LEU:HD23	1:C:139:LEU:HA	1.90	0.41
1:A:432:ALA:HB1	1:A:441:PRO:HG2	2.02	0.40
1:B:156:VAL:HG12	1:B:193:VAL:HG23	2.02	0.40
1:C:191:ASP:N	1:C:191:ASP:OD1	2.30	0.40
1:C:525:CYS:HA	1:C:540:LEU:O	2.20	0.40
1:B:208:ILE:HD12	1:B:208:ILE:HA	1.75	0.40
1:D:170:THR:O	1:D:179:MET:HG3	2.20	0.40
1:A:186:LEU:CD2	1:A:193:VAL:CG2	2.89	0.40
1:D:459:LEU:HA	1:D:459:LEU:HD23	1.84	0.40
1:B:182:LEU:HD23	1:B:182:LEU:HA	1.94	0.40
1:C:199:LEU:HA	1:C:199:LEU:HD12	1.86	0.40
1:C:411:LEU:HD23	1:C:411:LEU:HA	1.94	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:LYS:NZ	3:B:705:HOH:O[2_555]	1.97	0.23
1:A:307:ARG:NH2	1:B:259:ASP:OD1[1_455]	2.10	0.10

## 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	398/527 (76%)	388 (98%)	10 (2%)	0	100	100
1	B	407/527 (77%)	396 (97%)	11 (3%)	0	100	100
1	C	408/527 (77%)	397 (97%)	11 (3%)	0	100	100
1	D	407/527 (77%)	397 (98%)	10 (2%)	0	100	100
All	All	1620/2108 (77%)	1578 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	348/452 (77%)	344 (99%)	4 (1%)	73	89
1	B	354/452 (78%)	348 (98%)	6 (2%)	60	82
1	C	354/452 (78%)	347 (98%)	7 (2%)	55	79
1	D	354/452 (78%)	346 (98%)	8 (2%)	50	76
All	All	1410/1808 (78%)	1385 (98%)	25 (2%)	59	81

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	LYS
1	A	317	ARG
1	A	361	PHE
1	A	507	LYS
1	B	213	GLN
1	B	245	LYS
1	B	255	LYS
1	B	361	PHE
1	B	507	LYS
1	B	544	ARG
1	C	139	LEU
1	C	141	ASP
1	C	198	ASP

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Mol	Chain	Res	Type
1	C	205	GLN
1	C	255	LYS
1	C	361	PHE
1	C	507	LYS
1	D	186	LEU
1	D	216	ARG
1	D	242	SER
1	D	311	LYS
1	D	360	GLN
1	D	361	PHE
1	D	383	GLU
1	D	507	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	151	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	Q9M	D	601	1	29,39,39	2.24	7 (24%)	30,53,53	2.78	10 (33%)
2	Q9M	B	601	-	29,39,39	2.64	8 (27%)	30,53,53	2.40	10 (33%)

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	Q9M	D	601	1	-	0/14/32/32	0/5/5/5
2	Q9M	B	601	-	-	4/14/32/32	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	Q9M	C07-N08	8.33	1.45	1.32
2	D	601	Q9M	C07-N08	6.73	1.42	1.32
2	B	601	Q9M	C04-N03	5.82	1.46	1.36
2	D	601	Q9M	C04-N03	5.35	1.46	1.36
2	B	601	Q9M	C16-N17	5.11	1.45	1.36
2	D	601	Q9M	C02-N03	4.86	1.46	1.35
2	D	601	Q9M	C16-N17	4.66	1.44	1.36
2	B	601	Q9M	C18-N17	4.33	1.45	1.35
2	B	601	Q9M	O12-C13	3.82	1.41	1.36
2	B	601	Q9M	C02-N03	3.79	1.44	1.35
2	B	601	Q9M	O29-C02	-2.82	1.17	1.23
2	D	601	Q9M	O29-C02	-2.78	1.17	1.23
2	D	601	Q9M	C09-N08	2.66	1.50	1.47
2	B	601	Q9M	O26-C18	-2.43	1.18	1.23
2	D	601	Q9M	C11-N08	2.13	1.49	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	Q9M	C09-N08-C07	6.72	145.09	125.20
2	D	601	Q9M	C19-C18-N17	5.98	127.12	114.77
2	B	601	Q9M	C09-N08-C07	5.89	142.62	125.20
2	D	601	Q9M	C16-N17-C18	-5.31	115.19	129.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	Q9M	C04-N03-C02	-5.16	115.61	129.54
2	B	601	Q9M	C16-N17-C18	-5.02	115.97	129.54
2	D	601	Q9M	C04-N03-C02	-4.99	116.06	129.54
2	B	601	Q9M	C01-C02-N03	4.89	124.87	114.77
2	D	601	Q9M	C01-C02-N03	4.84	124.78	114.77
2	D	601	Q9M	O26-C18-C19	-4.37	112.09	122.03
2	D	601	Q9M	C30-C01-C02	-4.06	100.54	112.57
2	B	601	Q9M	C19-C18-N17	3.54	122.08	114.77
2	B	601	Q9M	O29-C02-C01	-3.04	115.12	122.03
2	D	601	Q9M	O29-C02-C01	-3.04	115.12	122.03
2	B	601	Q9M	C30-C01-C02	-2.69	104.60	112.57
2	B	601	Q9M	O26-C18-N17	-2.66	118.78	123.63
2	D	601	Q9M	O12-C10-C09	2.59	137.44	115.77
2	B	601	Q9M	O12-C10-C09	2.46	136.30	115.77
2	D	601	Q9M	C11-N08-C07	-2.30	118.38	125.20
2	B	601	Q9M	O29-C02-N03	-2.02	119.94	123.63

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	Q9M	C09-C10-O12-C13
2	B	601	Q9M	O26-C18-C19-C20
2	B	601	Q9M	C11-C10-O12-C13
2	B	601	Q9M	N17-C18-C19-C20

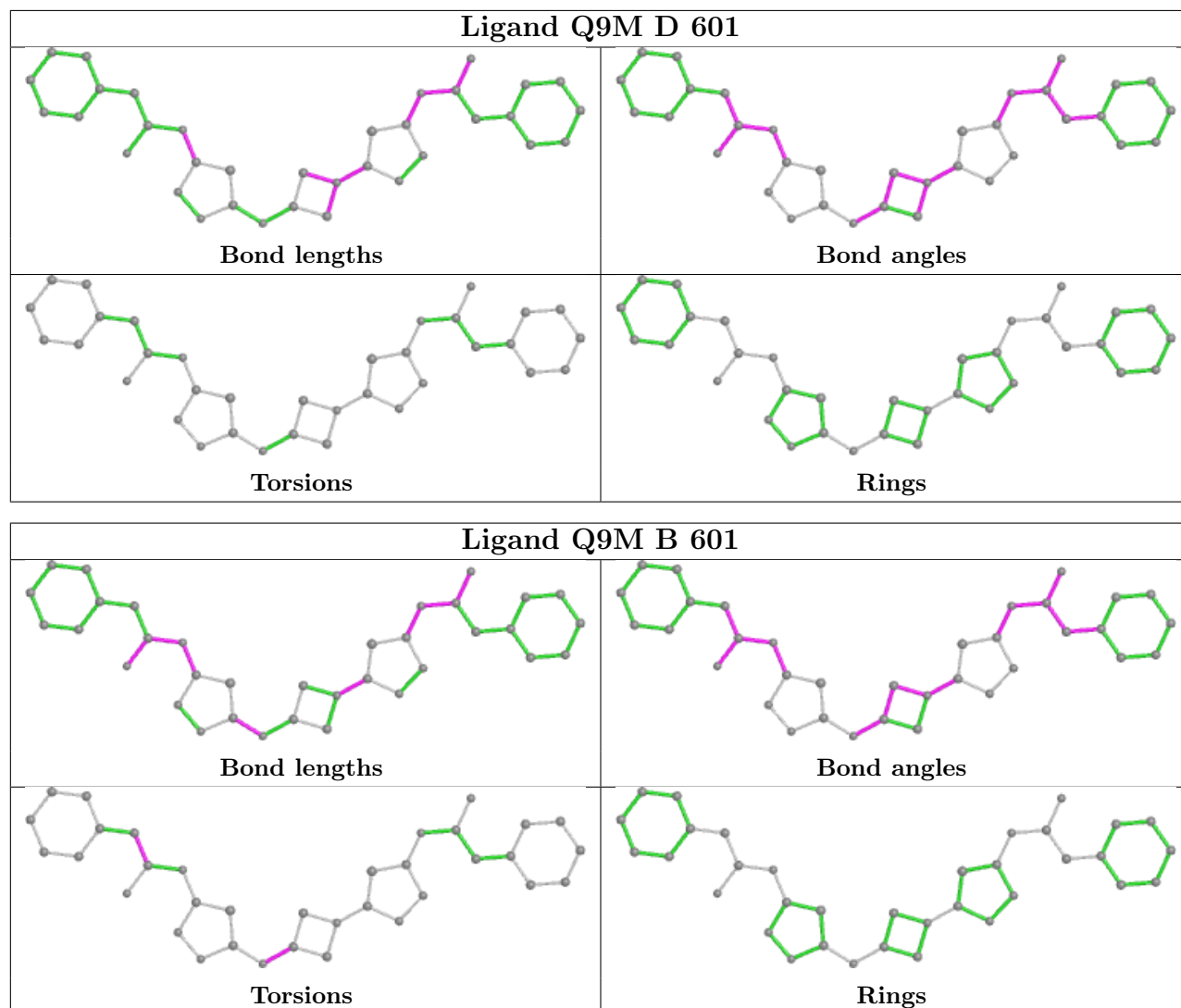
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	Q9M	1	0
2	B	601	Q9M	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	402/527 (76%)	0.47	38 (9%) 8 8	16, 27, 75, 174	0
1	B	409/527 (77%)	0.41	38 (9%) 8 8	16, 27, 72, 160	0
1	C	410/527 (77%)	0.47	50 (12%) 4 3	17, 27, 83, 132	0
1	D	409/527 (77%)	0.37	37 (9%) 9 9	17, 27, 71, 121	0
All	All	1630/2108 (77%)	0.43	163 (10%) 7 6	16, 27, 76, 174	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	189	THR	17.1
1	A	192	GLY	14.7
1	B	192	GLY	11.9
1	B	189	THR	9.8
1	A	191	ASP	9.5
1	B	191	ASP	9.1
1	D	318	PHE	7.2
1	B	318	PHE	7.1
1	D	137	PRO	6.8
1	A	148	ALA	6.5
1	A	190	SER	6.4
1	A	137	PRO	6.2
1	B	188	THR	6.1
1	D	195	LEU	6.0
1	D	144	PHE	5.9
1	B	150	GLY	5.8
1	B	148	ALA	5.8
1	C	316	LEU	5.8
1	B	145	TYR	5.5
1	B	190	SER	5.4
1	D	191	ASP	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	316	LEU	5.4
1	B	317	ARG	5.3
1	D	200	PHE	5.3
1	B	142	LEU	5.2
1	B	137	PRO	5.1
1	D	142	LEU	5.1
1	A	188	THR	5.1
1	A	186	LEU	5.1
1	D	156	VAL	4.9
1	D	150	GLY	4.9
1	C	142	LEU	4.8
1	C	546	GLY	4.8
1	B	186	LEU	4.8
1	A	317	ARG	4.8
1	A	318	PHE	4.7
1	A	150	GLY	4.7
1	C	317	ARG	4.7
1	A	249	TYR	4.7
1	D	317	ARG	4.6
1	D	192	GLY	4.6
1	A	145	TYR	4.6
1	C	252	GLN	4.5
1	B	144	PHE	4.5
1	B	149	GLU	4.5
1	A	195	LEU	4.4
1	D	193	VAL	4.4
1	C	150	GLY	4.3
1	B	154	ILE	4.3
1	A	257	SER	4.3
1	A	200	PHE	4.3
1	C	189	THR	4.3
1	C	192	GLY	4.2
1	A	193	VAL	4.2
1	B	193	VAL	4.2
1	B	195	LEU	4.1
1	B	200	PHE	4.1
1	A	258	PRO	4.1
1	B	146	THR	4.1
1	D	148	ALA	4.1
1	C	145	TYR	4.0
1	C	137	PRO	4.0
1	D	138	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	154	ILE	4.0
1	C	250	ILE	4.0
1	C	257	SER	4.0
1	B	147	ILE	4.0
1	D	152	GLU	4.0
1	C	152	GLU	3.9
1	B	141	ASP	3.9
1	C	144	PHE	3.8
1	D	204	VAL	3.8
1	A	149	GLU	3.8
1	A	147	ILE	3.8
1	C	138	SER	3.8
1	A	146	THR	3.8
1	C	256	PHE	3.7
1	D	154	ILE	3.7
1	C	198	ASP	3.7
1	A	152	GLU	3.6
1	C	139	LEU	3.6
1	D	149	GLU	3.6
1	C	253	LEU	3.5
1	B	196	ASP	3.5
1	B	160	ILE	3.5
1	B	156	VAL	3.5
1	C	258	PRO	3.5
1	A	154	ILE	3.4
1	C	318	PHE	3.4
1	C	249	TYR	3.4
1	D	199	LEU	3.4
1	C	193	VAL	3.4
1	C	199	LEU	3.3
1	D	139	LEU	3.3
1	C	203	CYS	3.3
1	D	151	GLN	3.3
1	C	148	ALA	3.3
1	B	143	LEU	3.3
1	B	251	PRO	3.2
1	B	197	LYS	3.2
1	C	156	VAL	3.2
1	C	251	PRO	3.2
1	A	185	THR	3.2
1	C	143	LEU	3.1
1	C	255	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	208	ILE	3.1
1	A	153	LYS	3.1
1	D	145	TYR	3.0
1	B	152	GLU	3.0
1	D	189	THR	3.0
1	A	187	GLN	3.0
1	D	208	ILE	3.0
1	A	142	LEU	3.0
1	A	143	LEU	2.9
1	C	149	GLU	2.9
1	C	348	GLY	2.9
1	C	206	SER	2.8
1	B	212	THR	2.7
1	A	197	LYS	2.7
1	D	146	THR	2.7
1	B	316	LEU	2.7
1	C	147	ILE	2.6
1	B	153	LYS	2.6
1	C	200	PHE	2.6
1	A	204	VAL	2.6
1	C	204	VAL	2.6
1	D	141	ASP	2.6
1	C	254	ALA	2.6
1	B	250	ILE	2.5
1	C	205	GLN	2.5
1	C	207	ASN	2.5
1	C	146	THR	2.5
1	B	138	SER	2.4
1	A	144	PHE	2.4
1	D	147	ILE	2.4
1	C	141	ASP	2.4
1	A	319	ASN	2.4
1	D	143	LEU	2.4
1	A	160	ILE	2.4
1	A	316	LEU	2.4
1	B	252	GLN	2.4
1	D	190	SER	2.4
1	C	216	ARG	2.4
1	C	158	LYS	2.3
1	D	215	PHE	2.3
1	A	184	LEU	2.3
1	B	199	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	138	SER	2.3
1	A	139	LEU	2.2
1	D	158	LYS	2.2
1	D	157	HIS	2.2
1	C	197	LYS	2.2
1	D	153	LYS	2.2
1	D	209	VAL	2.1
1	D	160	ILE	2.1
1	B	151	GLN	2.1
1	C	153	LYS	2.1
1	C	538	LYS	2.1
1	D	408	VAL	2.1
1	C	151	GLN	2.1
1	C	202	LYS	2.0
1	C	159	PHE	2.0
1	A	151	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

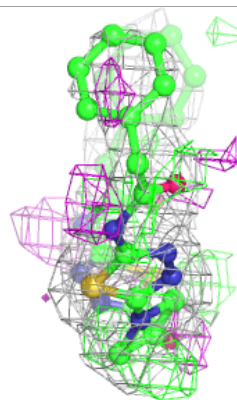
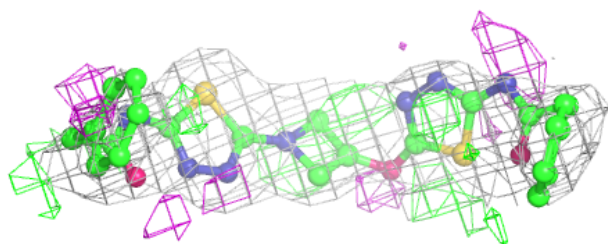
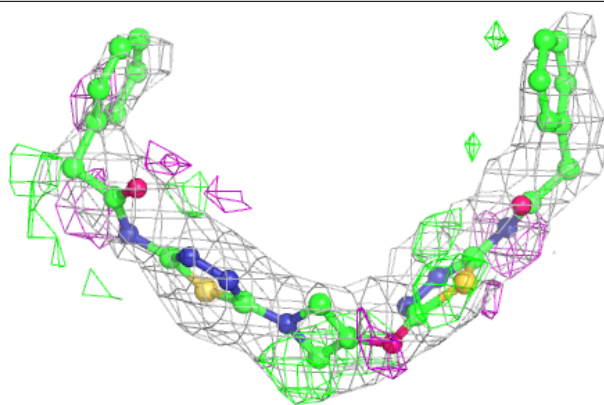
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	Q9M	D	601	35/35	0.83	0.28	35,62,72,74	0
2	Q9M	B	601	35/35	0.87	0.24	32,59,68,70	0

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.

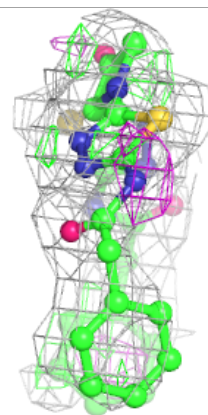
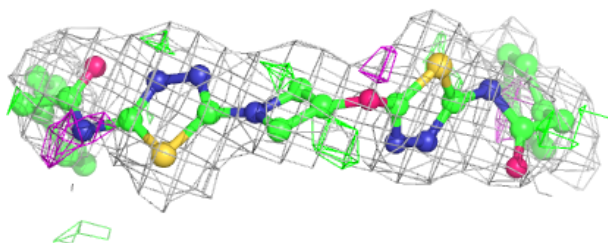
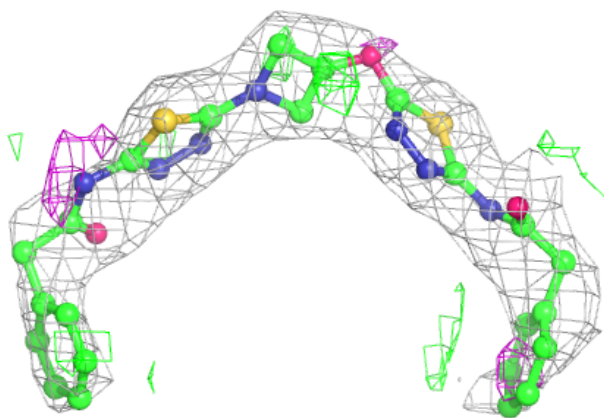


**Electron density around Q9M D 601:**

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

**Electron density around Q9M 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 [i](#)

There are no such residues in this entry.