



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2020 – 11:25 AM EDT

PDB ID : 6UMF
Title : Crystal structure of human GAC in complex with inhibitor UPGL00012
Authors : Huang, Q.; Cerione, R.A.
Deposited on : 2019-10-09
Resolution : 2.68 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 : 2.14.6
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

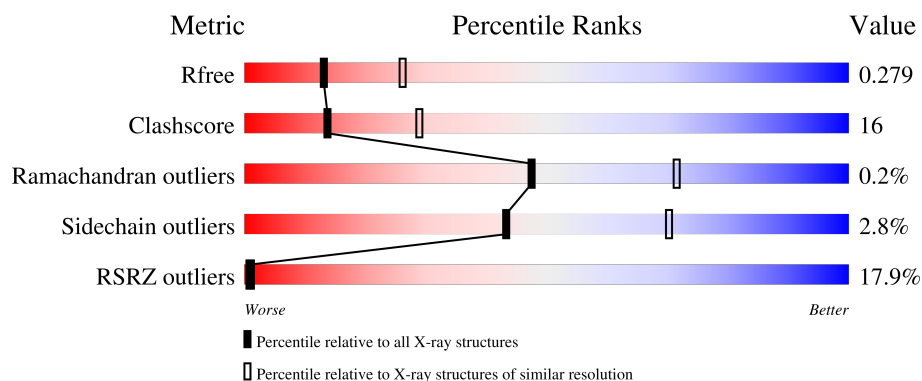
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	527	<div> <div>14%</div> <div> <div>54%</div> <div>22%</div> <div>•</div> <div>22%</div> </div> </div>
1	B	527	<div> <div>15%</div> <div> <div>54%</div> <div>23%</div> <div>•</div> <div>22%</div> </div> </div>
1	C	527	<div> <div>13%</div> <div> <div>55%</div> <div>21%</div> <div>•</div> <div>22%</div> </div> </div>
1	D	527	<div> <div>13%</div> <div> <div>50%</div> <div>26%</div> <div>•</div> <div>22%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12953 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

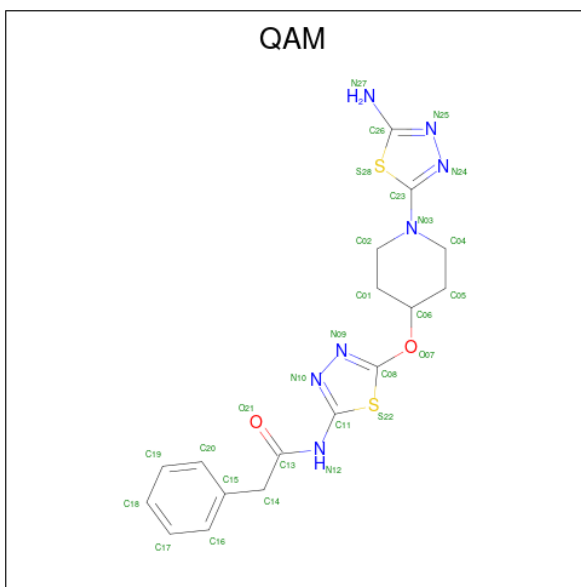
- Molecule 1 is a protein called Glutaminase kidney isoform, mitochondrial.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is N-(5-{[1-(5-amino-1,3,4-thiadiazol-2-yl)piperidin-4-yl]oxy}-1,3,4-thiadiazol-2-yl)-2-phenylacetamide (three-letter code: QAM) (formula: C₁₇H₁₉N₇O₂S₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total 28	C 17	N 7	O 2	S 2	0	0
2	C	1	Total 28	C 17	N 7	O 2	S 2	0	0

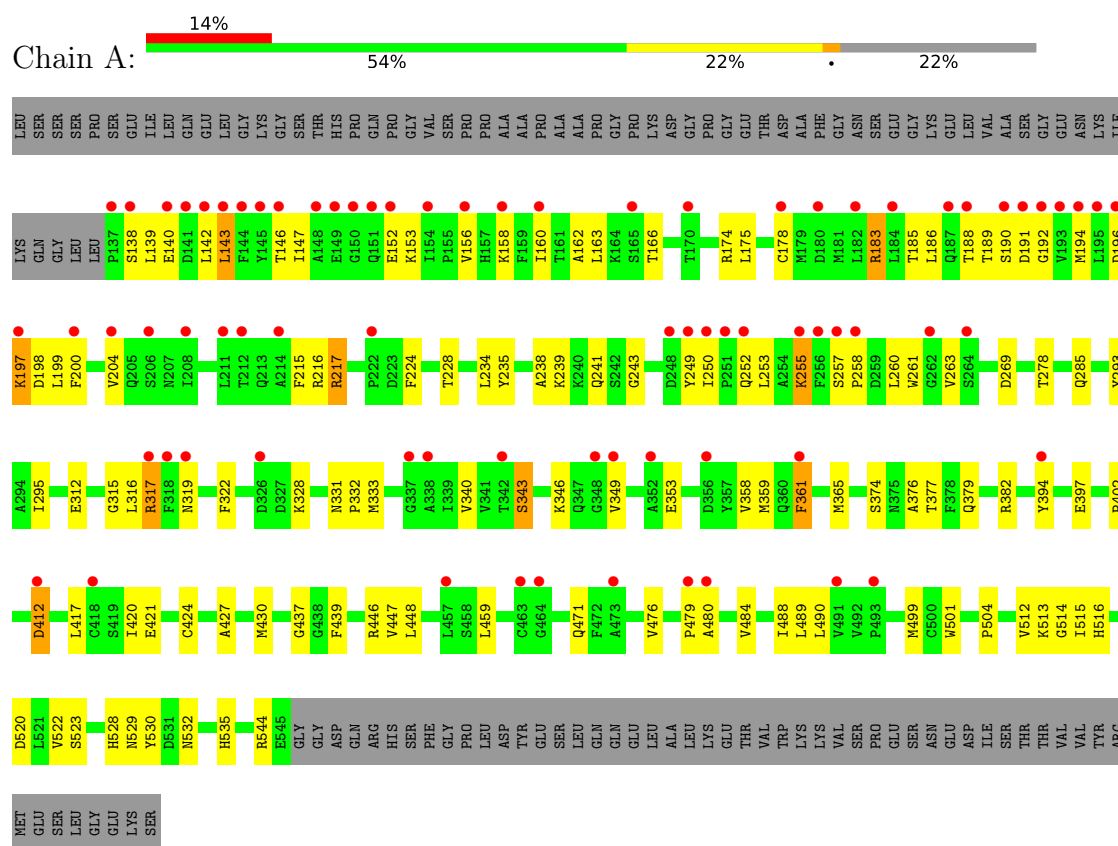
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	23	Total O 23 23	0	0
3	B	34	Total O 34 34	0	0
3	C	33	Total O 33 33	0	0
3	D	35	Total O 35 35	0	0

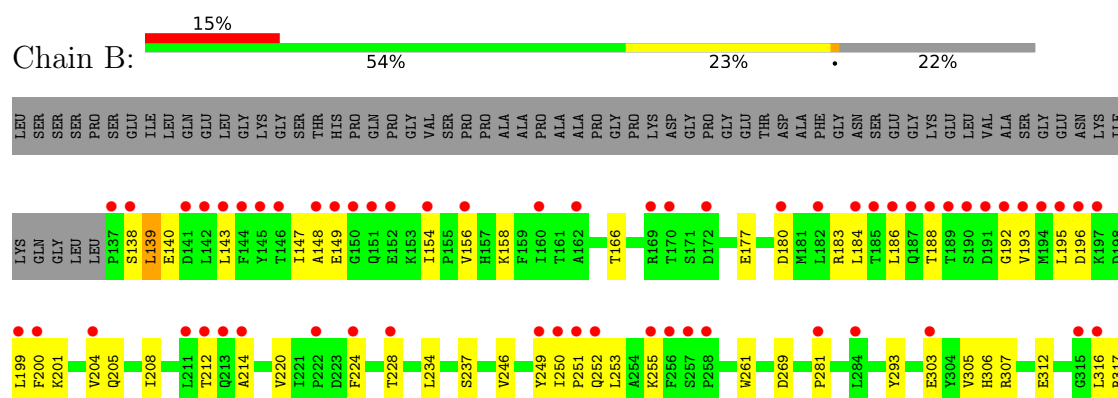
3 Residue-property plots

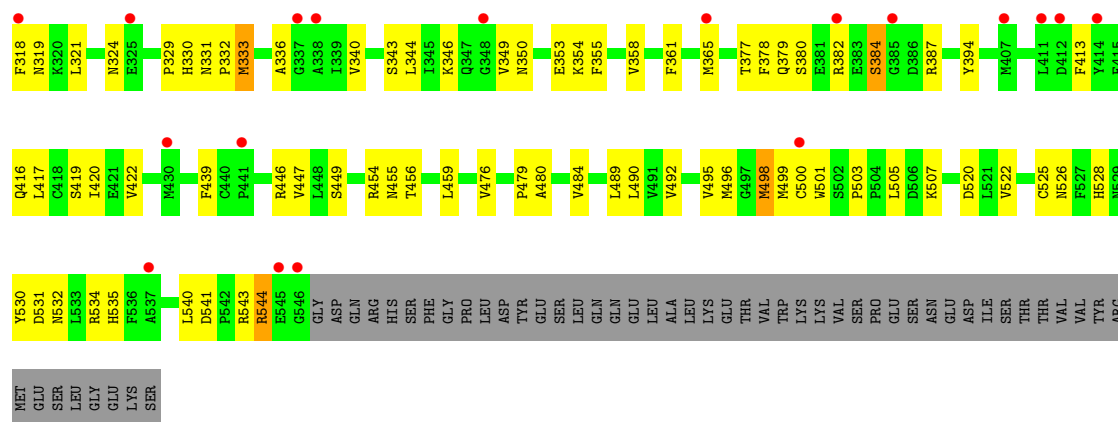
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

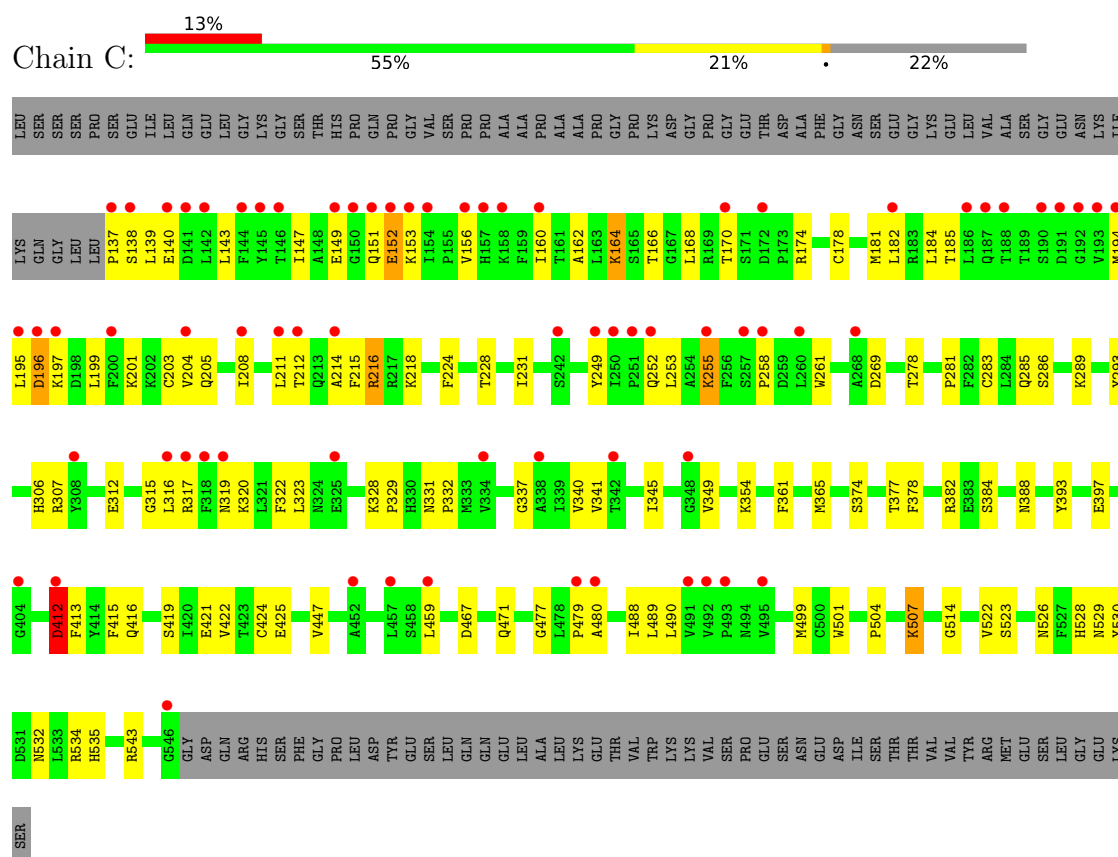


- Molecule 1: Glutaminase kidney isoform, mitochondrial

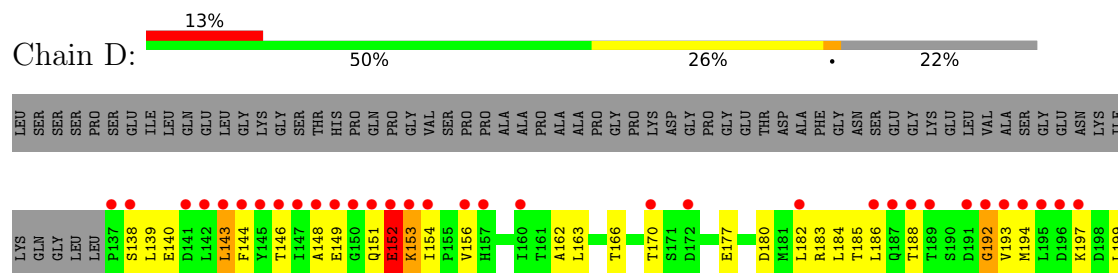


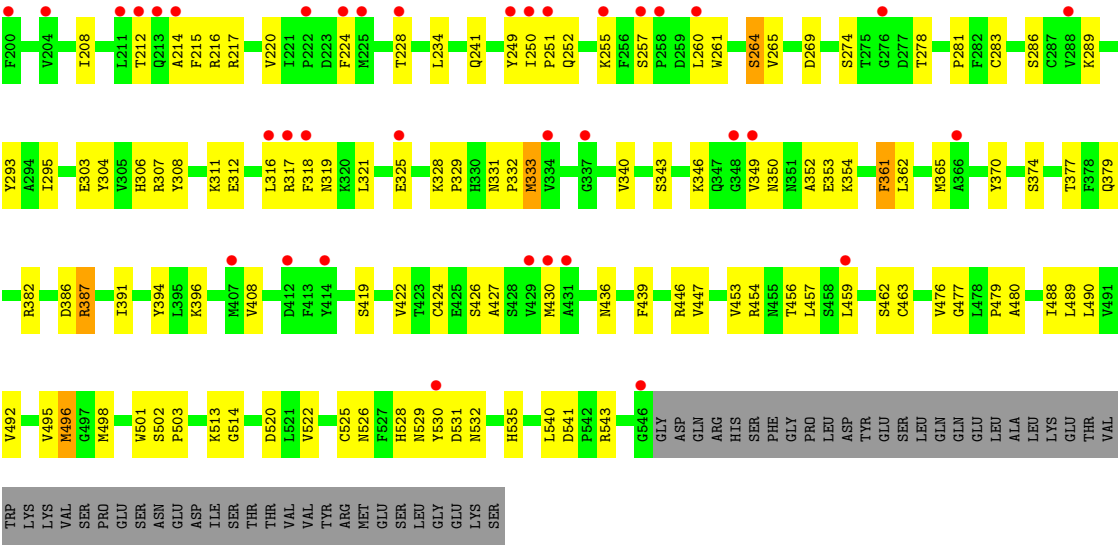


- Molecule 1: Glutaminase kidney isoform, mitochondrial



- 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	49.73Å 138.98Å 177.03Å 90.00° 93.91° 90.00°	Depositor
Resolution (Å)	48.64 – 2.68 48.64 – 2.68	Depositor EDS
% Data completeness (in resolution range)	92.0 (48.64-2.68) 92.0 (48.64-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.24	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.217 , 0.279 0.217 , 0.279	Depositor DCC
R_{free} test set	1949 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.696	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12953	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.49	0/3262	0.73	5/4403 (0.1%)
1	B	0.47	0/3266	0.70	1/4408 (0.0%)
1	C	0.52	0/3266	0.76	5/4408 (0.1%)
1	D	0.51	1/3266 (0.0%)	0.76	5/4408 (0.1%)
All	All	0.50	1/13060 (0.0%)	0.74	16/17627 (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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	152	GLU	CG-CD	-5.44	1.43	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	LEU	CB-CG-CD2	-10.66	92.88	111.00
1	D	143	LEU	CA-CB-CG	-10.47	91.23	115.30
1	D	199	LEU	CB-CG-CD2	-10.22	93.63	111.00
1	D	153	LYS	CA-CB-CG	8.92	133.02	113.40
1	D	143	LEU	CB-CG-CD2	8.72	125.82	111.00
1	A	190	SER	CA-C-N	-7.01	101.77	117.20
1	B	544	ARG	CB-CG-CD	-6.85	93.79	111.60
1	A	143	LEU	CB-CG-CD1	6.83	122.62	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	152	GLU	C-N-CA	6.29	137.43	121.70
1	A	217	ARG	NE-CZ-NH1	-6.09	117.25	120.30
1	C	139	LEU	CA-CB-CG	5.71	128.44	115.30
1	D	152	GLU	CB-CA-C	-5.69	99.03	110.40
1	C	152	GLU	CA-C-N	-5.50	105.09	117.20
1	C	412	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	A	217	ARG	CA-CB-CG	-5.24	101.87	113.40
1	C	197	LYS	CB-CG-CD	-5.16	98.20	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	152	GLU	Mainchain

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	3190	0	3167	106	0
1	B	3194	0	3170	103	0
1	C	3194	0	3170	93	0
1	D	3194	0	3170	122	0
2	B	28	0	0	3	0
2	C	28	0	0	4	0
3	A	23	0	0	12	0
3	B	34	0	0	2	0
3	C	33	0	0	4	0
3	D	35	0	0	6	0
All	All	12953	0	12677	405	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 16.

All (405) 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:317:ARG:NH2	1:D:325:GLU:OE1	1.78	1.14
1:B:250:ILE:HD11	1:B:253:LEU:HG	1.35	1.07
1:D:152:GLU:HG2	1:D:153:LYS:HD3	1.46	0.98
1:B:195:LEU:HD23	1:B:199:LEU:HG	1.53	0.91
1:D:153:LYS:HB3	1:D:194:MET:HB3	1.53	0.90
1:D:540:LEU:HD13	1:D:541:ASP:N	1.91	0.85
1:B:139:LEU:CD2	1:B:208:ILE:HG13	2.07	0.84
1:D:143:LEU:HD13	1:D:208:ILE:HD11	1.63	0.78
1:D:166:THR:HG21	1:D:214:ALA:HB1	1.66	0.78
1:A:166:THR:HA	1:A:217:ARG:HH12	1.50	0.76
1:A:471:GLN:HE22	1:D:311:LYS:HE3	1.51	0.75
1:B:318:PHE:HE1	1:C:317:ARG:HB2	1.50	0.75
1:D:143:LEU:HD13	1:D:212:THR:HG22	1.69	0.75
1:D:139:LEU:HD23	1:D:208:ILE:HG13	1.67	0.74
1:A:152:GLU:HG3	1:A:153:LYS:HG2	1.69	0.73
1:C:322:PHE:O	3:C:701:HOH:O	2.06	0.73
1:B:139:LEU:HD23	1:B:208:ILE:HG13	1.70	0.73
1:B:166:THR:HG21	1:B:214:ALA:HB1	1.70	0.73
1:C:164:LYS:HE3	1:C:170:THR:HG23	1.71	0.73
1:B:394:TYR:OH	2:B:601:QAM:S22	2.45	0.72
1:B:139:LEU:HD23	1:B:208:ILE:CG1	2.19	0.72
1:C:329:PRO:HG2	1:C:340:VAL:HG21	1.72	0.72
1:D:350:ASN:HD22	1:D:352:ALA:H	1.38	0.72
1:D:234:LEU:HD22	1:D:520:ASP:HB3	1.72	0.72
1:C:153:LYS:HG2	1:C:196:ASP:HB3	1.72	0.71
1:A:437:GLY:O	3:A:601:HOH:O	2.09	0.71
1:A:252:GLN:HB3	1:A:377:THR:HG22	1.73	0.70
1:B:382:ARG:NH1	3:B:701:HOH:O	2.10	0.70
1:D:346:LYS:HB3	1:D:354:LYS:HG2	1.73	0.69
1:A:189:THR:C	1:A:191:ASP:H	1.96	0.69
1:C:201:LYS:O	1:C:205:GLN:HB2	1.93	0.69
1:D:241:GLN:O	3:D:601:HOH:O	2.11	0.68
1:A:471:GLN:NE2	3:A:605:HOH:O	2.27	0.68
1:C:201:LYS:NZ	1:C:205:GLN:HG3	2.09	0.68
1:C:182:LEU:CD1	1:C:203:CYS:HB3	2.24	0.67
1:A:448:LEU:O	3:A:601:HOH:O	2.12	0.67
1:B:489:LEU:HD12	1:B:499:MET:HE2	1.75	0.67
1:B:234:LEU:HD22	1:B:520:ASP:HB3	1.75	0.66
1:A:178:CYS:SG	1:A:204:VAL:HG12	2.36	0.66
1:C:153:LYS:HB2	1:C:194:MET:HG2	1.79	0.65
1:A:382:ARG:NH2	1:A:412:ASP:OD2	2.29	0.65
1:B:186:LEU:HD23	1:B:193:VAL:HG11	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:601:QAM:S22	1:D:394:TYR:OH	2.55	0.65
1:C:382:ARG:NH1	3:C:703:HOH:O	2.27	0.65
1:B:143:LEU:HD23	1:B:200:PHE:HZ	1.63	0.64
1:D:139:LEU:HG	1:D:143:LEU:HD11	1.79	0.64
1:D:333:MET:HE2	1:D:333:MET:N	2.12	0.64
1:A:312:GLU:OE1	1:D:316:LEU:HD22	1.97	0.64
1:D:374:SER:OG	1:D:377:THR:HG23	1.99	0.63
1:B:333:MET:CE	1:B:459:LEU:HB3	2.29	0.62
1:A:146:THR:HG21	1:A:216:ARG:HH21	1.64	0.62
1:D:152:GLU:CG	1:D:153:LYS:HD3	2.26	0.62
1:B:317:ARG:NH2	1:B:319:ASN:HD21	1.97	0.62
1:B:490:LEU:HD23	1:B:498:MET:HE2	1.82	0.62
1:D:340:VAL:O	1:D:343:SER:OG	2.13	0.62
1:D:261:TRP:HB2	1:D:513:LYS:HE3	1.82	0.62
1:A:258:PRO:HB3	1:A:504:PRO:HG3	1.83	0.61
1:C:216:ARG:O	1:C:218:LYS:HG2	1.99	0.61
1:B:251:PRO:O	1:B:255:LYS:HG3	2.00	0.61
2:B:601:QAM:C18	1:C:317:ARG:HG3	2.31	0.61
1:D:396:LYS:NZ	3:D:606:HOH:O	2.32	0.61
1:A:319:ASN:N	3:A:602:HOH:O	2.33	0.60
1:D:526:ASN:OD1	1:D:543:ARG:NH2	2.33	0.60
1:B:148:ALA:O	1:B:149:GLU:HB2	2.01	0.60
1:A:185:THR:HG21	1:A:199:LEU:HD11	1.82	0.60
1:B:180:ASP:OD1	1:B:183:ARG:NH1	2.34	0.60
1:C:278:THR:HA	1:C:424:CYS:HB2	1.82	0.60
1:D:163:LEU:HD23	1:D:170:THR:HG22	1.83	0.60
1:B:252:GLN:CB	1:B:377:THR:HG22	2.32	0.60
1:B:318:PHE:HE1	1:C:317:ARG:CB	2.12	0.60
1:C:382:ARG:NH2	1:C:412:ASP:OD2	2.35	0.60
1:A:143:LEU:CD2	1:A:200:PHE:HZ	2.14	0.59
1:A:544:ARG:NH1	1:A:544:ARG:HA	2.17	0.59
1:C:174:ARG:NH1	1:C:269:ASP:O	2.33	0.59
1:A:349:VAL:CG1	1:A:353:GLU:HB2	2.32	0.59
1:A:471:GLN:HG2	3:D:618:HOH:O	2.02	0.59
1:D:252:GLN:HB3	1:D:377:THR:HG22	1.84	0.59
1:B:250:ILE:HG13	1:B:253:LEU:H	1.69	0.58
1:A:140:GLU:OE1	1:A:140:GLU:N	2.32	0.58
1:A:317:ARG:HB3	1:D:318:PHE:HE2	1.67	0.58
1:B:340:VAL:O	1:B:343:SER:HB3	2.03	0.58
1:D:251:PRO:O	1:D:255:LYS:HG3	2.03	0.58
1:C:201:LYS:HZ1	1:C:205:GLN:HG3	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:LEU:O	1:C:147:ILE:HD12	2.04	0.58
1:A:224:PHE:O	1:A:228:THR:HG23	2.03	0.57
1:A:139:LEU:H	1:A:139:LEU:HD12	1.68	0.57
1:B:252:GLN:HB3	1:B:377:THR:HG22	1.87	0.57
1:B:139:LEU:CD2	1:B:208:ILE:CG1	2.80	0.57
1:B:143:LEU:HD23	1:B:200:PHE:CZ	2.39	0.57
1:C:253:LEU:HD21	1:C:285:GLN:HE21	1.69	0.57
1:A:529:ASN:OD1	1:D:529:ASN:ND2	2.31	0.57
1:C:166:THR:OG1	1:C:168:LEU:HD12	2.05	0.57
1:D:319:ASN:N	3:D:602:HOH:O	2.21	0.57
1:D:208:ILE:O	1:D:212:THR:HG23	2.05	0.57
1:C:195:LEU:HA	1:C:199:LEU:HD23	1.85	0.56
1:D:143:LEU:CD1	1:D:208:ILE:HD11	2.35	0.56
1:A:427:ALA:HA	1:A:430:MET:HG3	1.87	0.56
1:C:522:VAL:CG1	1:C:528:HIS:HB2	2.35	0.56
1:B:147:ILE:O	1:B:158:LYS:NZ	2.39	0.56
1:D:148:ALA:O	1:D:149:GLU:HB2	2.06	0.56
1:C:143:LEU:HD11	1:C:212:THR:CG2	2.36	0.56
1:A:138:SER:O	1:A:142:LEU:HD22	2.06	0.55
1:D:139:LEU:O	1:D:143:LEU:HD12	2.05	0.55
1:D:332:PRO:HD2	1:D:459:LEU:HD13	1.88	0.55
1:B:332:PRO:HD2	1:B:459:LEU:HD13	1.86	0.55
1:D:177:GLU:H	1:D:177:GLU:CD	2.10	0.55
1:D:332:PRO:C	1:D:333:MET:HE2	2.26	0.55
1:C:178:CYS:SG	1:C:204:VAL:HG12	2.46	0.55
1:D:332:PRO:HB2	1:D:333:MET:HE2	1.89	0.55
1:D:143:LEU:HD13	1:D:212:THR:CG2	2.34	0.55
1:C:143:LEU:CD1	1:C:208:ILE:HD11	2.36	0.54
1:C:182:LEU:HD12	1:C:203:CYS:SG	2.47	0.54
1:A:471:GLN:NE2	1:D:311:LYS:HE3	2.20	0.54
1:C:204:VAL:HB	1:C:211:LEU:HD13	1.89	0.54
1:C:293:TYR:OH	1:C:306:HIS:NE2	2.35	0.54
1:C:365:MET:HG3	1:C:447:VAL:HG11	1.89	0.54
1:B:480:ALA:HB2	1:B:490:LEU:HD12	1.90	0.54
1:D:362:LEU:HD22	1:D:430:MET:HE1	1.89	0.54
1:D:365:MET:HG3	1:D:447:VAL:HG11	1.90	0.54
1:B:261:TRP:HA	1:B:501:TRP:O	2.07	0.53
1:A:479:PRO:HG3	1:D:530:TYR:CE1	2.42	0.53
1:A:379:GLN:O	1:A:382:ARG:HG2	2.09	0.53
1:C:252:GLN:HB3	1:C:377:THR:HG22	1.89	0.53
1:B:349:VAL:O	1:B:354:LYS:HE3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:SER:O	1:A:142:LEU:CD2	2.56	0.53
1:A:544:ARG:HH11	1:A:544:ARG:HA	1.73	0.53
1:B:140:GLU:CB	1:B:201:LYS:HG3	2.38	0.53
1:C:153:LYS:HB3	1:C:195:LEU:C	2.28	0.53
1:C:480:ALA:HB2	1:C:490:LEU:HD12	1.90	0.53
1:B:417:LEU:HD23	1:B:420:ILE:HD11	1.91	0.53
1:A:257:SER:O	1:A:260:LEU:HD12	2.09	0.53
1:D:257:SER:O	1:D:503:PRO:HG2	2.08	0.53
1:C:522:VAL:HG11	1:C:528:HIS:HB2	1.90	0.53
1:B:476:VAL:HG13	1:B:522:VAL:HG21	1.91	0.53
1:A:476:VAL:HG13	1:A:522:VAL:HG21	1.91	0.52
1:C:185:THR:HG21	1:C:199:LEU:HD11	1.90	0.52
1:A:143:LEU:HD22	1:A:200:PHE:HZ	1.73	0.52
1:B:365:MET:HG3	1:B:447:VAL:HG11	1.91	0.52
1:C:345:ILE:HD11	1:C:413:PHE:CE2	2.44	0.52
1:A:250:ILE:HD11	1:A:253:LEU:HG	1.92	0.52
1:A:143:LEU:CD2	1:A:200:PHE:CZ	2.93	0.52
1:A:489:LEU:HD12	1:A:499:MET:HE2	1.91	0.52
1:C:374:SER:HB2	1:C:421:GLU:OE2	2.08	0.52
1:C:507:LYS:H	1:C:507:LYS:HD3	1.74	0.52
1:D:156:VAL:HG21	1:D:186:LEU:HD11	1.90	0.52
1:A:480:ALA:HB2	1:A:490:LEU:HD12	1.92	0.52
1:B:148:ALA:HA	1:B:154:ILE:HD13	1.91	0.52
1:C:332:PRO:HD2	1:C:459:LEU:HD13	1.92	0.52
1:C:374:SER:OG	1:C:377:THR:HG23	2.10	0.52
1:C:283:CYS:HB3	1:C:419:SER:HA	1.91	0.52
1:B:324:ASN:HB3	1:B:330:HIS:CD2	2.45	0.52
1:C:377:THR:OG1	1:C:419:SER:HB3	2.10	0.52
1:A:530:TYR:CE1	1:D:479:PRO:HG3	2.45	0.52
1:B:147:ILE:O	1:B:149:GLU:HG2	2.09	0.52
1:B:303:GLU:OE2	1:B:307:ARG:NH1	2.43	0.51
1:D:436:ASN:ND2	3:D:611:HOH:O	2.43	0.51
1:A:147:ILE:O	1:A:158:LYS:NZ	2.44	0.51
1:A:528:HIS:CD2	1:D:454:ARG:HD2	2.45	0.51
1:A:484:VAL:HG12	3:A:606:HOH:O	2.10	0.51
1:D:265:VAL:HG22	1:D:498:MET:HE2	1.93	0.51
1:C:149:GLU:OE1	1:C:151:GLN:HG3	2.11	0.51
1:D:162:ALA:HB1	1:D:215:PHE:HE1	1.74	0.51
1:A:512:VAL:N	3:A:607:HOH:O	2.43	0.51
1:A:239:LYS:HA	1:A:513:LYS:HD3	1.93	0.51
1:B:379:GLN:O	1:B:382:ARG:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:GLU:HG2	1:C:149:GLU:O	2.11	0.51
1:A:332:PRO:HD2	1:A:459:LEU:HD13	1.93	0.50
1:C:312:GLU:O	1:C:331:ASN:ND2	2.43	0.50
1:A:162:ALA:HB1	1:A:215:PHE:HE1	1.76	0.50
1:D:143:LEU:CD1	1:D:212:THR:CG2	2.88	0.50
1:B:329:PRO:HG2	1:B:340:VAL:HG21	1.92	0.50
1:A:359:MET:SD	1:A:420:ILE:HD12	2.51	0.50
1:B:439:PHE:CE2	1:B:446:ARG:HB2	2.47	0.50
1:A:358:VAL:HG11	1:A:417:LEU:HD22	1.93	0.50
1:B:177:GLU:H	1:B:177:GLU:CD	2.15	0.50
1:D:281:PRO:HA	1:D:422:VAL:O	2.12	0.50
1:A:261:TRP:HA	1:A:501:TRP:O	2.11	0.50
1:B:140:GLU:HB2	1:B:201:LYS:HG3	1.94	0.50
1:C:216:ARG:NE	3:C:708:HOH:O	2.45	0.50
1:C:477:GLY:O	1:C:529:ASN:HB2	2.12	0.50
1:D:143:LEU:CD1	1:D:212:THR:HG22	2.40	0.50
1:B:378:PHE:CE1	1:B:416:GLN:HG3	2.47	0.50
1:B:349:VAL:HG23	1:B:354:LYS:HG3	1.93	0.50
1:D:488:ILE:HD12	1:D:514:GLY:HA3	1.94	0.50
1:A:374:SER:OG	1:A:377:THR:HG23	2.12	0.49
1:A:252:GLN:NE2	1:A:376:ALA:O	2.45	0.49
1:B:530:TYR:CE1	1:C:479:PRO:HG3	2.47	0.49
1:C:258:PRO:HB3	1:C:504:PRO:HG3	1.94	0.49
1:B:333:MET:HE2	1:B:459:LEU:HB3	1.94	0.49
1:D:387:ARG:HD3	1:D:391:ILE:HD11	1.94	0.49
1:D:148:ALA:O	1:D:151:GLN:HB2	2.12	0.49
1:A:488:ILE:HD12	1:A:514:GLY:HA3	1.94	0.49
1:C:156:VAL:O	1:C:160:ILE:HG12	2.12	0.49
1:A:315:GLY:O	3:A:602:HOH:O	2.18	0.49
1:A:183:ARG:HA	1:A:186:LEU:HB2	1.95	0.49
1:D:350:ASN:HD22	1:D:352:ALA:N	2.06	0.49
1:D:453:VAL:HG12	1:D:457:LEU:HD11	1.95	0.49
1:B:380:SER:O	1:B:384:SER:HB3	2.13	0.49
1:C:153:LYS:HB3	1:C:195:LEU:O	2.12	0.49
1:C:143:LEU:HD12	1:C:208:ILE:HD11	1.95	0.49
1:A:397:GLU:HG3	1:B:387:ARG:HB2	1.94	0.49
1:C:162:ALA:HB1	1:C:215:PHE:HE1	1.78	0.49
1:D:312:GLU:O	1:D:331:ASN:ND2	2.45	0.49
1:D:462:SER:HB2	1:D:463:CYS:SG	2.53	0.49
1:A:252:GLN:CB	1:A:377:THR:HG22	2.42	0.48
1:C:489:LEU:HD12	1:C:499:MET:HE2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:488:ILE:HD12	1:C:514:GLY:HA3	1.94	0.48
1:D:249:TYR:CD2	1:D:250:ILE:HG23	2.48	0.48
1:D:349:VAL:O	1:D:354:LYS:HE3	2.13	0.48
1:C:143:LEU:HD11	1:C:212:THR:HG22	1.95	0.48
1:D:408:VAL:O	3:D:603:HOH:O	2.20	0.48
1:D:532:ASN:HB3	1:D:535:HIS:O	2.13	0.48
1:A:315:GLY:C	1:A:317:ARG:H	2.16	0.48
1:C:316:LEU:HD21	1:C:467:ASP:HB3	1.96	0.48
1:C:397:GLU:OE1	1:D:386:ASP:HB2	2.13	0.48
1:A:439:PHE:CE2	1:A:446:ARG:HB2	2.49	0.48
1:D:283:CYS:SG	1:D:419:SER:HA	2.53	0.48
1:A:513:LYS:HG3	3:A:615:HOH:O	2.12	0.48
1:B:312:GLU:OE2	1:C:471:GLN:NE2	2.46	0.48
1:C:315:GLY:O	1:C:317:ARG:N	2.47	0.48
1:D:261:TRP:HA	1:D:501:TRP:O	2.14	0.48
1:A:239:LYS:HG2	1:A:239:LYS:O	2.14	0.48
1:A:374:SER:HB2	1:A:421:GLU:OE2	2.14	0.48
1:D:143:LEU:HD11	1:D:212:THR:HG21	1.95	0.48
1:D:293:TYR:OH	1:D:306:HIS:NE2	2.33	0.48
1:A:189:THR:OG1	1:A:191:ASP:HB3	2.14	0.48
1:D:139:LEU:HD21	1:D:212:THR:HG21	1.96	0.47
1:D:502:SER:OG	1:D:513:LYS:HE2	2.14	0.47
1:B:143:LEU:O	1:B:147:ILE:HG22	2.14	0.47
1:C:393:TYR:OH	3:C:702:HOH:O	2.20	0.47
1:C:526:ASN:OD1	1:C:543:ARG:NH2	2.47	0.47
1:C:278:THR:O	1:C:425:GLU:HG3	2.14	0.47
1:B:358:VAL:HG11	1:B:417:LEU:HD22	1.97	0.47
1:A:317:ARG:HD3	2:C:601:QAM:C19	2.44	0.47
1:D:540:LEU:HD13	1:D:541:ASP:C	2.35	0.47
1:A:153:LYS:CD	1:A:196:ASP:HB3	2.44	0.47
1:A:315:GLY:O	1:A:317:ARG:N	2.48	0.47
1:D:525:CYS:HA	1:D:540:LEU:O	2.13	0.47
1:B:249:TYR:HE1	1:B:484:VAL:HG11	1.79	0.47
1:D:303:GLU:HG2	1:D:304:TYR:N	2.29	0.47
1:B:526:ASN:OD1	1:B:543:ARG:NH2	2.48	0.47
1:B:281:PRO:HA	1:B:422:VAL:O	2.14	0.47
1:B:319:ASN:OD1	1:B:319:ASN:N	2.48	0.46
1:B:261:TRP:HZ3	1:B:500:CYS:HB3	1.80	0.46
1:C:166:THR:HG21	1:C:214:ALA:HB1	1.97	0.46
1:D:192:GLY:HA3	1:D:193:VAL:HA	1.64	0.46
1:A:174:ARG:NH1	1:A:269:ASP:O	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:LEU:HD22	1:B:208:ILE:CD1	2.46	0.46
1:B:350:ASN:HD21	1:B:353:GLU:HG3	1.80	0.46
1:D:332:PRO:CD	1:D:459:LEU:HD13	2.44	0.46
1:A:156:VAL:O	1:A:160:ILE:HG12	2.15	0.46
1:A:241:GLN:HG3	1:A:516:HIS:CG	2.51	0.46
1:A:319:ASN:N	1:A:319:ASN:OD1	2.44	0.46
1:A:343:SER:OG	1:A:402:PRO:HD2	2.15	0.46
1:C:224:PHE:O	1:C:228:THR:HG23	2.15	0.46
1:D:252:GLN:CB	1:D:377:THR:HG22	2.46	0.46
1:B:261:TRP:CZ3	1:B:500:CYS:HB3	2.50	0.46
1:D:332:PRO:CB	1:D:333:MET:HE2	2.46	0.46
1:B:140:GLU:HG3	1:B:208:ILE:HG12	1.97	0.46
1:D:152:GLU:HB3	1:D:153:LYS:H	1.48	0.46
1:B:143:LEU:HD13	1:B:212:THR:OG1	2.16	0.46
1:D:293:TYR:HD2	1:D:456:THR:HG1	1.64	0.46
1:B:489:LEU:HB2	1:B:499:MET:HE1	1.98	0.46
1:C:319:ASN:HB3	1:C:467:ASP:OD1	2.16	0.46
1:D:140:GLU:HG3	1:D:208:ILE:HG12	1.96	0.46
1:D:286:SER:O	1:D:289:LYS:HG3	2.16	0.46
1:D:264:SER:HB3	1:D:424:CYS:HB3	1.98	0.46
1:A:349:VAL:HG11	1:A:353:GLU:HB2	1.98	0.45
1:B:479:PRO:HG3	1:C:530:TYR:CE1	2.51	0.45
1:A:253:LEU:HD21	1:A:285:GLN:HE21	1.80	0.45
1:B:454:ARG:HD3	1:C:528:HIS:CD2	2.51	0.45
1:D:260:LEU:HD13	1:D:501:TRP:CH2	2.51	0.45
1:C:140:GLU:N	1:C:140:GLU:OE1	2.34	0.45
1:C:143:LEU:HD21	1:C:212:THR:HG22	1.98	0.45
1:B:355:PHE:HD2	1:B:413:PHE:HE1	1.64	0.45
1:B:455:ASN:HD22	1:B:455:ASN:N	2.14	0.45
1:B:507:LYS:HD3	1:B:507:LYS:HA	1.50	0.45
1:A:340:VAL:O	1:A:343:SER:HB3	2.17	0.45
1:C:137:PRO:O	1:C:138:SER:HB3	2.16	0.45
1:A:234:LEU:CD2	1:A:520:ASP:HB3	2.47	0.45
1:C:281:PRO:HA	1:C:422:VAL:O	2.16	0.45
1:B:220:VAL:N	1:B:269:ASP:OD2	2.48	0.45
1:B:312:GLU:O	1:B:331:ASN:ND2	2.47	0.45
1:C:412:ASP:OD1	1:C:416:GLN:OE1	2.35	0.45
1:B:249:TYR:CD2	1:B:250:ILE:HG23	2.52	0.45
1:D:308:TYR:HB3	1:D:340:VAL:CG1	2.46	0.45
1:D:350:ASN:ND2	1:D:353:GLU:H	2.15	0.45
1:B:336:ALA:O	1:B:340:VAL:HG23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:ARG:HD2	1:B:535:HIS:NE2	2.33	0.44
1:C:337:GLY:O	1:C:341:VAL:HG23	2.17	0.44
1:D:308:TYR:O	1:D:329:PRO:HD2	2.17	0.44
1:B:358:VAL:HG11	1:B:417:LEU:CD2	2.47	0.44
1:B:544:ARG:HA	1:B:544:ARG:HD2	1.42	0.44
1:C:322:PHE:C	1:C:323:LEU:HD23	2.38	0.44
1:B:246:VAL:HG22	1:B:503:PRO:HB2	2.00	0.44
1:B:318:PHE:CE1	1:C:317:ARG:HB2	2.41	0.44
1:D:480:ALA:HB2	1:D:490:LEU:HD12	1.98	0.44
1:A:185:THR:HA	1:A:188:THR:OG1	2.18	0.44
1:A:153:LYS:HB2	1:A:194:MET:SD	2.58	0.44
1:D:332:PRO:HB2	1:D:333:MET:CE	2.46	0.44
1:D:422:VAL:HG21	1:D:427:ALA:HB2	2.00	0.44
1:A:295:ILE:HG12	1:A:361:PHE:CD2	2.52	0.44
1:B:377:THR:OG1	1:B:419:SER:HB3	2.17	0.44
1:D:307:ARG:O	1:D:328:LYS:HE2	2.17	0.44
1:D:379:GLN:O	1:D:382:ARG:HG2	2.18	0.44
1:D:490:LEU:HB3	1:D:498:MET:HB3	1.99	0.44
1:B:350:ASN:ND2	1:B:353:GLU:HG3	2.32	0.44
1:B:293:TYR:HD2	1:B:456:THR:HG1	1.65	0.44
1:B:495:VAL:HG22	1:B:543:ARG:HD3	1.99	0.44
1:C:252:GLN:CB	1:C:377:THR:HG22	2.47	0.44
1:D:308:TYR:HB3	1:D:340:VAL:HG11	1.99	0.44
1:A:529:ASN:CG	1:D:529:ASN:HD21	2.21	0.44
1:A:238:ALA:HA	1:A:516:HIS:CD2	2.52	0.44
1:D:220:VAL:HG21	1:D:495:VAL:HA	2.00	0.44
1:D:439:PHE:CE2	1:D:446:ARG:HB2	2.52	0.44
1:A:235:TYR:CE1	1:A:261:TRP:CD1	3.05	0.43
1:A:315:GLY:C	1:A:317:ARG:N	2.72	0.43
1:B:532:ASN:HB3	1:B:535:HIS:O	2.18	0.43
1:C:143:LEU:HD11	1:C:212:THR:HG23	2.00	0.43
1:B:528:HIS:HB3	1:B:531:ASP:OD2	2.18	0.43
1:C:286:SER:O	1:C:289:LYS:HG3	2.18	0.43
1:C:534:ARG:HD2	1:C:535:HIS:CE1	2.53	0.43
1:A:365:MET:HG3	1:A:447:VAL:HG11	2.00	0.43
1:B:224:PHE:O	1:B:228:THR:HG23	2.18	0.43
1:B:293:TYR:HE1	1:B:305:VAL:HG11	1.84	0.43
1:C:231:ILE:HA	1:C:231:ILE:HD13	1.77	0.43
1:D:224:PHE:O	1:D:228:THR:HG23	2.18	0.43
1:D:350:ASN:HD21	1:D:352:ALA:HB3	1.83	0.43
1:A:189:THR:O	1:A:189:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LYS:NZ	3:A:610:HOH:O	2.52	0.43
1:B:484:VAL:O	1:B:505:LEU:HD11	2.17	0.43
1:D:180:ASP:OD1	1:D:183:ARG:NH2	2.52	0.43
1:A:143:LEU:HD22	1:A:200:PHE:CZ	2.53	0.43
1:A:322:PHE:O	3:A:603:HOH:O	2.21	0.43
1:D:146:THR:HG21	1:D:216:ARG:HH12	1.84	0.42
1:D:149:GLU:HB2	1:D:151:GLN:HB2	2.00	0.42
1:D:182:LEU:O	1:D:186:LEU:HD13	2.19	0.42
1:D:295:ILE:HG12	1:D:361:PHE:CG	2.54	0.42
1:A:532:ASN:HB3	1:A:535:HIS:O	2.19	0.42
1:C:307:ARG:O	1:C:328:LYS:HE2	2.19	0.42
1:D:144:PHE:CD2	1:D:197:LYS:HG3	2.54	0.42
1:D:370:TYR:O	1:D:426:SER:OG	2.25	0.42
1:A:278:THR:HA	1:A:424:CYS:HB2	2.01	0.42
1:A:480:ALA:HA	1:A:489:LEU:O	2.19	0.42
1:D:495:VAL:HG12	1:D:496:MET:HB3	2.01	0.42
1:A:358:VAL:HG11	1:A:417:LEU:CD2	2.50	0.42
1:B:156:VAL:HG23	1:B:195:LEU:HD11	2.02	0.42
2:C:601:QAM:N10	1:D:321:LEU:HD22	2.35	0.42
1:A:249:TYR:CD2	1:A:250:ILE:HG23	2.54	0.42
1:B:346:LYS:HB3	1:B:354:LYS:HG2	2.01	0.42
1:C:153:LYS:HG2	1:C:196:ASP:CB	2.45	0.42
1:B:200:PHE:O	1:B:204:VAL:HG22	2.20	0.42
1:B:318:PHE:CD2	1:B:321:LEU:HD13	2.54	0.42
1:B:344:LEU:O	3:B:702:HOH:O	2.22	0.42
1:C:345:ILE:HD11	1:C:413:PHE:HE2	1.84	0.42
1:B:332:PRO:CD	1:B:459:LEU:HD13	2.50	0.42
1:C:532:ASN:HB3	1:C:535:HIS:O	2.19	0.42
1:A:312:GLU:O	1:A:331:ASN:ND2	2.48	0.42
1:B:140:GLU:OE2	1:B:205:GLN:HG3	2.20	0.42
1:B:492:VAL:HG21	1:B:496:MET:HE3	2.02	0.42
1:D:185:THR:HA	1:D:188:THR:HG23	2.02	0.41
1:D:260:LEU:HD13	1:D:501:TRP:HH2	1.84	0.41
1:B:148:ALA:O	1:B:149:GLU:CB	2.66	0.41
1:D:148:ALA:HA	1:D:154:ILE:CG2	2.49	0.41
1:C:320:LYS:HZ3	2:C:601:QAM:C16	2.33	0.41
1:D:261:TRP:CD1	1:D:513:LYS:HD2	2.55	0.41
1:C:255:LYS:O	1:C:255:LYS:HG2	2.20	0.41
1:C:349:VAL:O	1:C:354:LYS:HE3	2.20	0.41
1:C:261:TRP:HA	1:C:501:TRP:O	2.19	0.41
1:D:274:SER:HB3	1:D:278:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:477:GLY:O	1:D:529:ASN:HB2	2.19	0.41
1:A:175:LEU:HD23	1:A:175:LEU:HA	1.85	0.41
1:B:540:LEU:HD23	1:B:541:ASP:N	2.35	0.41
1:A:143:LEU:HD11	1:A:215:PHE:CD2	2.56	0.41
1:D:144:PHE:O	1:D:148:ALA:HB2	2.21	0.41
1:A:235:TYR:HD1	1:A:263:VAL:HG23	1.86	0.41
1:B:293:TYR:OH	1:B:306:HIS:NE2	2.33	0.41
1:D:143:LEU:CD1	1:D:212:THR:HG21	2.50	0.41
1:D:346:LYS:O	1:D:354:LYS:HE2	2.19	0.41
1:D:492:VAL:HG21	1:D:496:MET:CE	2.51	0.41
1:B:184:LEU:O	1:B:188:THR:HG23	2.20	0.41
1:B:166:THR:CG2	1:B:214:ALA:HB1	2.45	0.41
1:D:522:VAL:CG1	1:D:528:HIS:HB2	2.51	0.41
1:A:197:LYS:HB3	1:A:197:LYS:HE3	1.85	0.41
1:A:243:GLY:O	1:A:512:VAL:HG21	2.21	0.41
1:D:528:HIS:HB3	1:D:531:ASP:OD1	2.20	0.41
1:A:394:TYR:CE1	2:B:601:QAM:C04	3.04	0.41
1:B:316:LEU:HA	1:B:316:LEU:HD23	1.81	0.41
1:D:184:LEU:HD23	1:D:184:LEU:HA	1.81	0.41
1:D:476:VAL:HG13	1:D:522:VAL:HG21	2.02	0.41
1:A:515:ILE:HB	3:A:621:HOH:O	2.21	0.40
1:B:446:ARG:NH2	1:B:449:SER:HB3	2.36	0.40
1:C:316:LEU:HD23	1:C:316:LEU:HA	1.68	0.40
1:C:378:PHE:HZ	1:C:412:ASP:OD1	2.04	0.40
1:C:388:ASN:HD22	1:C:415:PHE:HE1	1.70	0.40
1:D:220:VAL:N	1:D:269:ASP:OD2	2.50	0.40
1:A:153:LYS:CB	1:A:194:MET:HG2	2.52	0.40
1:A:293:TYR:CE2	1:A:459:LEU:HD12	2.55	0.40
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.85	0.40
1:C:332:PRO:CD	1:C:459:LEU:HD13	2.51	0.40
1:A:163:LEU:HD12	1:A:163:LEU:HA	1.85	0.40
1:A:346:LYS:N	3:A:611:HOH:O	2.55	0.40
1:A:255:LYS:HB3	1:A:255:LYS:HE3	1.95	0.40
1:B:525:CYS:HA	1:B:540:LEU:O	2.22	0.40
1:C:315:GLY:C	1:C:317:ARG:H	2.24	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	407/527 (77%)	396 (97%)	10 (2%)	1 (0%)	47	71
1	B	408/527 (77%)	393 (96%)	14 (3%)	1 (0%)	47	71
1	C	408/527 (77%)	395 (97%)	12 (3%)	1 (0%)	47	71
1	D	408/527 (77%)	391 (96%)	16 (4%)	1 (0%)	47	71
All	All	1631/2108 (77%)	1575 (97%)	52 (3%)	4 (0%)	47	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	152	GLU
1	A	192	GLY
1	B	192	GLY
1	D	192	GLY

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	353/451 (78%)	343 (97%)	10 (3%)	43	70
1	B	353/451 (78%)	345 (98%)	8 (2%)	50	76
1	C	353/451 (78%)	341 (97%)	12 (3%)	37	63
1	D	353/451 (78%)	344 (98%)	9 (2%)	47	74
All	All	1412/1804 (78%)	1373 (97%)	39 (3%)	43	70

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

Mol	Chain	Res	Type
1	A	183	ARG
1	A	197	LYS
1	A	198	ASP
1	A	255	LYS
1	A	317	ARG
1	A	333	MET
1	A	343	SER
1	A	361	PHE
1	A	412	ASP
1	A	523	SER
1	B	138	SER
1	B	139	LEU
1	B	196	ASP
1	B	237	SER
1	B	333	MET
1	B	361	PHE
1	B	384	SER
1	B	498	MET
1	C	164	LYS
1	C	181	MET
1	C	184	LEU
1	C	196	ASP
1	C	216	ARG
1	C	249	TYR
1	C	255	LYS
1	C	361	PHE
1	C	384	SER
1	C	412	ASP
1	C	507	LYS
1	C	523	SER
1	D	138	SER
1	D	217	ARG
1	D	264	SER
1	D	317	ARG
1	D	333	MET
1	D	361	PHE
1	D	387	ARG
1	D	489	LEU
1	D	496	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
1	A	285	GLN
1	A	471	GLN
1	A	516	HIS
1	A	519	HIS
1	B	230	HIS
1	B	330	HIS
1	B	510	ASN
1	C	285	GLN
1	C	388	ASN
1	C	416	GLN
1	C	519	HIS
1	C	535	HIS
1	D	330	HIS
1	D	350	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 monosaccharides 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	QAM	B	601	-	23,31,31	2.92	8 (34%)	21,42,42	2.12	3 (14%)
2	QAM	C	601	-	23,31,31	2.93	7 (30%)	21,42,42	1.33	4 (19%)

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	QAM	B	601	-	-	4/10/26/26	0/4/4/4
2	QAM	C	601	-	-	4/10/26/26	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	QAM	C23-N03	7.87	1.44	1.32
2	B	601	QAM	C23-N03	7.54	1.44	1.32
2	C	601	QAM	C11-N12	5.32	1.46	1.36
2	C	601	QAM	C02-N03	5.31	1.55	1.46
2	B	601	QAM	C04-N03	5.20	1.54	1.46
2	B	601	QAM	C13-N12	5.19	1.47	1.35
2	B	601	QAM	C11-N12	5.14	1.45	1.36
2	C	601	QAM	C13-N12	5.10	1.46	1.35
2	B	601	QAM	C02-N03	5.00	1.54	1.46
2	C	601	QAM	C04-N03	4.55	1.53	1.46
2	B	601	QAM	C26-N27	3.80	1.46	1.35
2	C	601	QAM	C26-N27	3.54	1.45	1.35
2	C	601	QAM	O07-C08	2.80	1.40	1.36
2	B	601	QAM	O07-C08	2.43	1.39	1.36
2	B	601	QAM	C01-C06	-2.30	1.44	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	QAM	C02-C01-C06	-6.67	102.98	110.32
2	B	601	QAM	O07-C06-C05	4.18	117.56	108.31
2	B	601	QAM	C11-N12-C13	-2.80	121.99	129.54
2	C	601	QAM	C11-N12-C13	-2.73	122.17	129.54
2	C	601	QAM	C14-C13-N12	2.57	120.07	114.77
2	C	601	QAM	C05-C06-C01	-2.26	107.39	111.74
2	C	601	QAM	C04-C05-C06	-2.15	107.95	110.32

There are no chirality outliers.

All (8) torsion outliers are listed below:

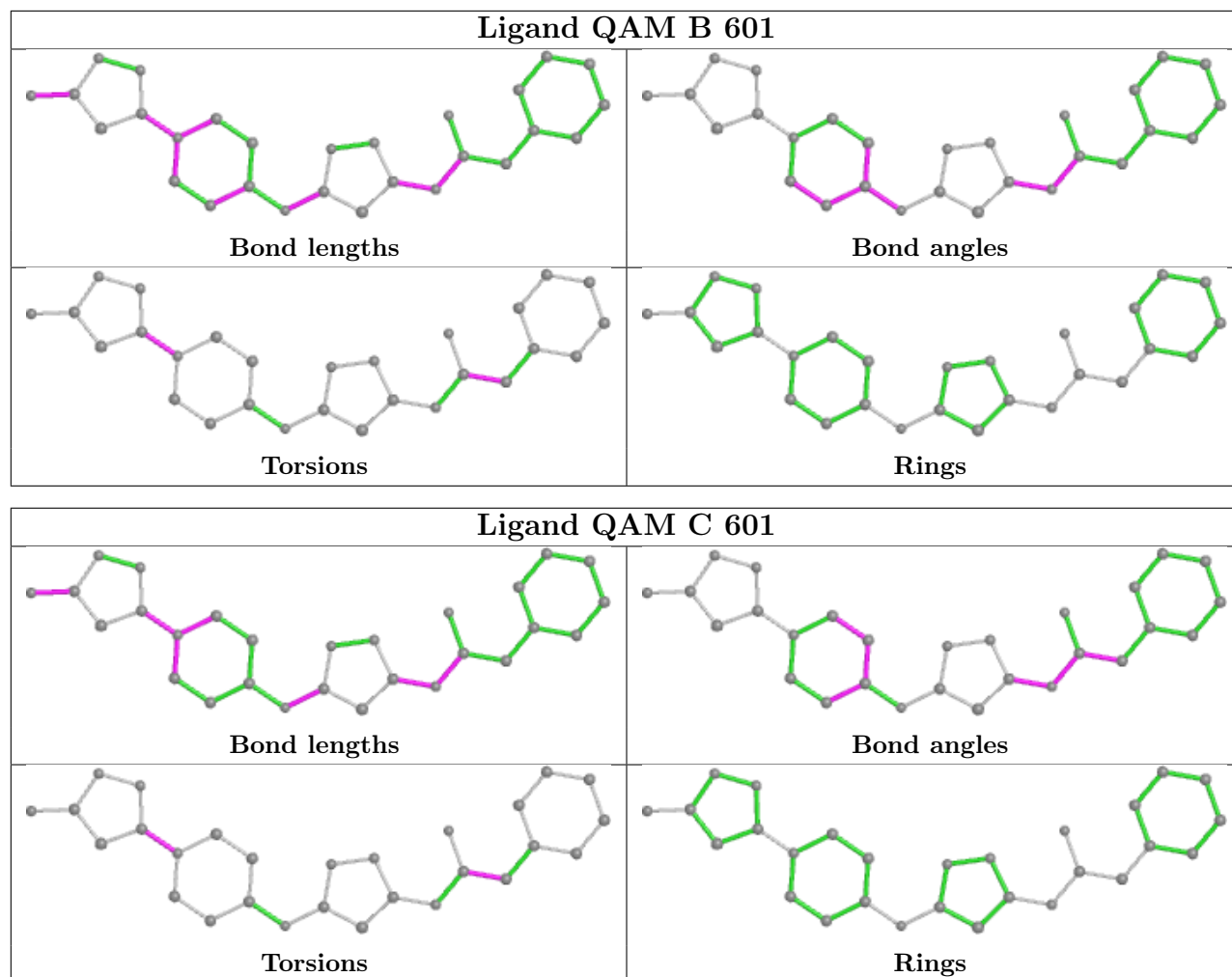
Mol	Chain	Res	Type	Atoms
2	B	601	QAM	S28-C23-N03-C02
2	B	601	QAM	S28-C23-N03-C04
2	C	601	QAM	S28-C23-N03-C02
2	C	601	QAM	S28-C23-N03-C04
2	B	601	QAM	O21-C13-C14-C15
2	C	601	QAM	O21-C13-C14-C15
2	B	601	QAM	N12-C13-C14-C15
2	C	601	QAM	N12-C13-C14-C15

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	QAM	3	0
2	C	601	QAM	4	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	409/527 (77%)	1.18	76 (18%)  	31, 52, 96, 157	0
1	B	410/527 (77%)	1.26	77 (18%)  	30, 51, 102, 169	0
1	C	410/527 (77%)	1.13	70 (17%)  	26, 48, 97, 137	0
1	D	410/527 (77%)	1.16	70 (17%)  	25, 49, 94, 164	0
All	All	1639/2108 (77%)	1.18	293 (17%)  	25, 50, 97, 169	0

All (293) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	192	GLY	18.6
1	B	192	GLY	14.3
1	C	144	PHE	10.5
1	B	191	ASP	10.2
1	A	144	PHE	9.7
1	B	189	THR	9.5
1	C	195	LEU	8.9
1	A	191	ASP	8.8
1	C	192	GLY	8.8
1	D	195	LEU	8.5
1	B	144	PHE	8.2
1	A	252	GLN	8.1
1	C	251	PRO	7.6
1	C	252	GLN	7.5
1	D	144	PHE	7.4
1	B	200	PHE	7.2
1	B	188	THR	7.2
1	B	250	ILE	7.2
1	B	195	LEU	7.1
1	B	318	PHE	7.0
1	D	318	PHE	6.9

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Mol	Chain	Res	Type	RSRZ
1	D	200	PHE	6.9
1	D	191	ASP	6.9
1	D	188	THR	6.7
1	B	149	GLU	6.7
1	B	148	ALA	6.6
1	A	250	ILE	6.6
1	C	193	VAL	6.6
1	D	189	THR	6.5
1	D	150	GLY	6.5
1	D	193	VAL	6.4
1	B	146	THR	6.4
1	A	255	LYS	6.4
1	A	142	LEU	6.3
1	D	142	LEU	6.3
1	A	251	PRO	6.2
1	D	196	ASP	6.2
1	C	142	LEU	6.1
1	C	412	ASP	6.1
1	A	195	LEU	5.9
1	C	255	LYS	5.8
1	D	211	LEU	5.8
1	C	318	PHE	5.8
1	B	337	GLY	5.7
1	B	160	ILE	5.7
1	B	251	PRO	5.7
1	B	211	LEU	5.6
1	A	257	SER	5.6
1	B	142	LEU	5.4
1	B	348	GLY	5.4
1	D	317	ARG	5.3
1	B	258	PRO	5.3
1	A	318	PHE	5.3
1	C	191	ASP	5.1
1	C	194	MET	5.1
1	D	228	THR	5.1
1	A	150	GLY	5.1
1	B	150	GLY	5.1
1	D	348	GLY	5.1
1	A	182	LEU	4.9
1	D	250	ILE	4.9
1	C	149	GLU	4.9
1	B	186	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	213	GLN	4.8
1	C	200	PHE	4.8
1	C	319	ASN	4.7
1	C	138	SER	4.6
1	A	211	LEU	4.5
1	A	256	PHE	4.5
1	B	137	PRO	4.5
1	C	250	ILE	4.5
1	A	156	VAL	4.4
1	A	193	VAL	4.4
1	A	319	ASN	4.4
1	D	148	ALA	4.4
1	D	212	THR	4.4
1	C	546	GLY	4.4
1	D	337	GLY	4.3
1	B	156	VAL	4.2
1	D	149	GLU	4.2
1	A	196	ASP	4.2
1	D	197	LYS	4.2
1	B	196	ASP	4.2
1	D	249	TYR	4.1
1	A	160	ILE	4.1
1	B	193	VAL	4.1
1	A	348	GLY	4.0
1	C	137	PRO	4.0
1	C	152	GLU	4.0
1	D	224	PHE	4.0
1	D	146	THR	4.0
1	D	213	GLN	4.0
1	B	145	TYR	4.0
1	B	224	PHE	4.0
1	D	137	PRO	4.0
1	D	152	GLU	4.0
1	A	249	TYR	3.9
1	D	258	PRO	3.9
1	C	156	VAL	3.9
1	A	194	MET	3.9
1	A	148	ALA	3.9
1	B	143	LEU	3.9
1	B	249	TYR	3.9
1	C	211	LEU	3.9
1	B	257	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	151	GLN	3.9
1	D	430	MET	3.9
1	B	170	THR	3.8
1	A	138	SER	3.8
1	B	185	THR	3.8
1	C	196	ASP	3.8
1	C	146	THR	3.8
1	A	192	GLY	3.7
1	C	190	SER	3.7
1	D	255	LYS	3.7
1	C	214	ALA	3.7
1	D	160	ILE	3.7
1	B	212	THR	3.7
1	B	338	ALA	3.7
1	C	145	TYR	3.7
1	C	342	THR	3.7
1	A	342	THR	3.6
1	B	204	VAL	3.6
1	B	152	GLU	3.6
1	A	143	LEU	3.5
1	B	252	GLN	3.5
1	B	325	GLU	3.5
1	D	156	VAL	3.5
1	C	157	HIS	3.5
1	A	338	ALA	3.5
1	C	151	GLN	3.5
1	D	412	ASP	3.5
1	C	257	SER	3.5
1	D	147	ILE	3.5
1	C	204	VAL	3.4
1	C	249	TYR	3.4
1	A	146	THR	3.4
1	A	180	ASP	3.4
1	B	414	TYR	3.4
1	D	204	VAL	3.4
1	D	138	SER	3.4
1	C	212	THR	3.4
1	B	182	LEU	3.3
1	D	145	TYR	3.3
1	C	188	THR	3.3
1	D	186	LEU	3.3
1	C	404	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	214	ALA	3.3
1	A	151	GLN	3.3
1	A	137	PRO	3.3
1	A	141	ASP	3.3
1	C	316	LEU	3.2
1	C	348	GLY	3.2
1	D	170	THR	3.2
1	C	317	ARG	3.2
1	A	158	LYS	3.2
1	D	194	MET	3.2
1	B	255	LYS	3.2
1	A	184	LEU	3.2
1	D	172	ASP	3.1
1	C	150	GLY	3.1
1	A	149	GLU	3.1
1	A	200	PHE	3.1
1	A	356	ASP	3.1
1	B	172	ASP	3.1
1	D	157	HIS	3.0
1	A	165	SER	3.0
1	C	479	PRO	3.0
1	D	251	PRO	3.0
1	D	325	GLU	3.0
1	B	214	ALA	3.0
1	A	214	ALA	3.0
1	A	145	TYR	3.0
1	A	170	THR	2.9
1	A	206	SER	2.9
1	B	546	GLY	2.9
1	B	190	SER	2.9
1	D	459	LEU	2.9
1	B	187	GLN	2.9
1	B	407	MET	2.9
1	A	326	ASP	2.9
1	A	412	ASP	2.9
1	C	153	LYS	2.9
1	C	154	ILE	2.8
1	B	228	THR	2.8
1	C	308	TYR	2.8
1	B	382	ARG	2.8
1	B	194	MET	2.8
1	A	204	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	412	ASP	2.7
1	D	407	MET	2.7
1	D	153	LYS	2.7
1	D	334	VAL	2.7
1	D	225	MET	2.7
1	C	186	LEU	2.7
1	B	141	ASP	2.7
1	A	394	TYR	2.7
1	A	258	PRO	2.7
1	B	197	LYS	2.7
1	C	459	LEU	2.7
1	C	140	GLU	2.7
1	C	480	ALA	2.7
1	D	546	GLY	2.7
1	B	430	MET	2.7
1	B	316	LEU	2.7
1	A	337	GLY	2.6
1	B	385	GLY	2.6
1	A	361	PHE	2.6
1	B	169	ARG	2.6
1	A	187	GLN	2.6
1	D	316	LEU	2.6
1	B	151	GLN	2.6
1	A	190	SER	2.6
1	D	222	PRO	2.6
1	C	182	LEU	2.6
1	B	184	LEU	2.6
1	B	411	LEU	2.5
1	C	334	VAL	2.5
1	C	492	VAL	2.5
1	C	258	PRO	2.5
1	C	197	LYS	2.5
1	A	317	ARG	2.5
1	D	141	ASP	2.5
1	D	429	VAL	2.5
1	A	152	GLU	2.5
1	C	141	ASP	2.5
1	A	479	PRO	2.5
1	A	212	THR	2.4
1	A	222	PRO	2.4
1	A	493	PRO	2.4
1	B	256	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	188	THR	2.4
1	D	366	ALA	2.4
1	A	154	ILE	2.4
1	D	154	ILE	2.4
1	A	491	VAL	2.3
1	C	158	LYS	2.3
1	A	480	ALA	2.3
1	C	260	LEU	2.3
1	D	276	GLY	2.3
1	C	338	ALA	2.3
1	C	325	GLU	2.3
1	C	172	ASP	2.3
1	A	248	ASP	2.3
1	B	138	SER	2.3
1	B	199	LEU	2.3
1	B	162	ALA	2.3
1	A	208	ILE	2.3
1	C	208	ILE	2.3
1	D	349	VAL	2.3
1	A	140	GLU	2.2
1	B	303	GLU	2.2
1	D	143	LEU	2.2
1	A	352	ALA	2.2
1	A	473	ALA	2.2
1	B	537	ALA	2.2
1	D	187	GLN	2.2
1	C	268	ALA	2.2
1	D	288	VAL	2.2
1	D	260	LEU	2.2
1	C	495	VAL	2.2
1	C	187	GLN	2.2
1	B	154	ILE	2.2
1	D	182	LEU	2.2
1	B	365	MET	2.2
1	D	530	TYR	2.2
1	C	160	ILE	2.2
1	C	491	VAL	2.2
1	B	222	PRO	2.2
1	C	493	PRO	2.2
1	A	418	CYS	2.2
1	D	431	ALA	2.2
1	C	452	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	178	CYS	2.1
1	A	464	GLY	2.1
1	D	257	SER	2.1
1	B	315	GLY	2.1
1	A	197	LYS	2.1
1	B	180	ASP	2.1
1	A	457	LEU	2.1
1	B	545	GLU	2.1
1	B	441	PRO	2.1
1	C	170	THR	2.1
1	D	414	TYR	2.0
1	A	463	CYS	2.0
1	A	262	GLY	2.0
1	B	284	LEU	2.0
1	C	457	LEU	2.0
1	A	349	VAL	2.0
1	A	264	SER	2.0
1	B	500	CYS	2.0
1	B	281	PRO	2.0
1	C	242	SER	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](#)

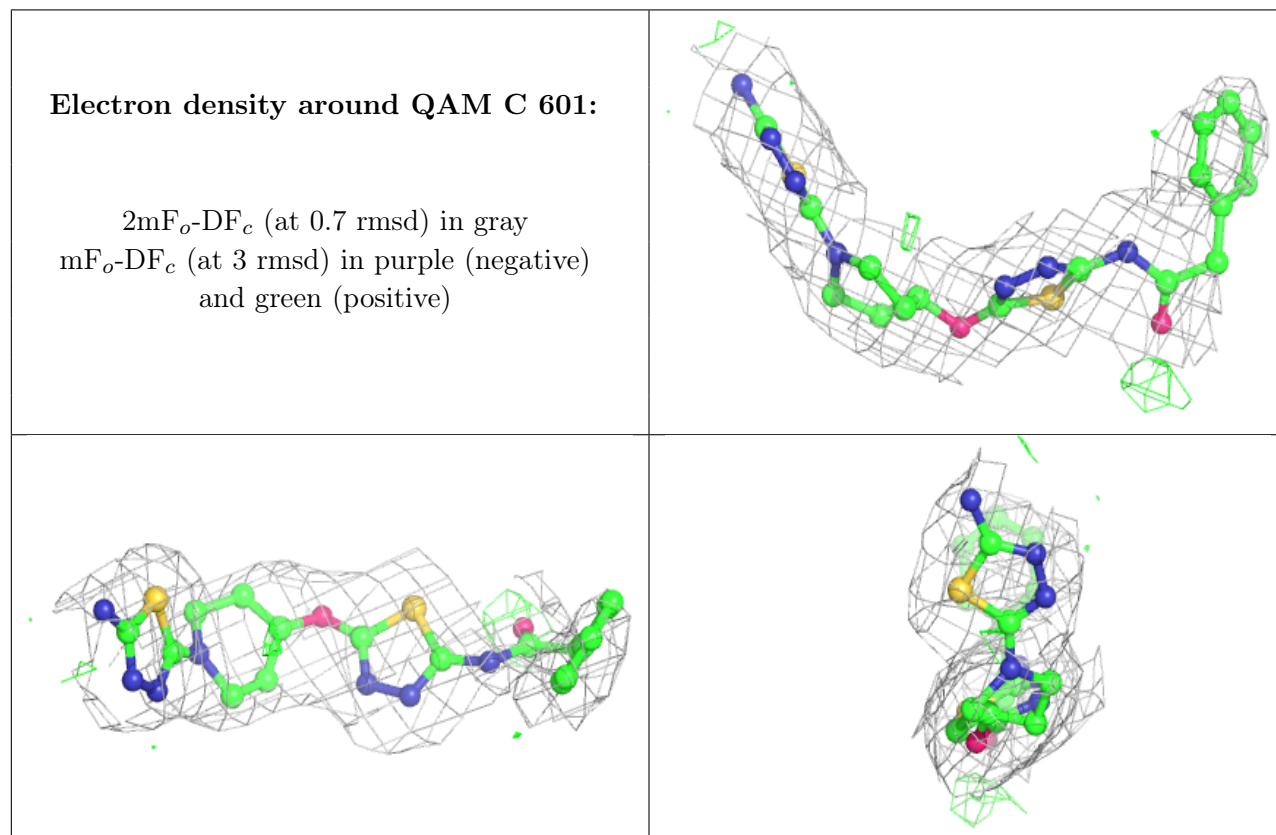
There are no monosaccharides in this entry.

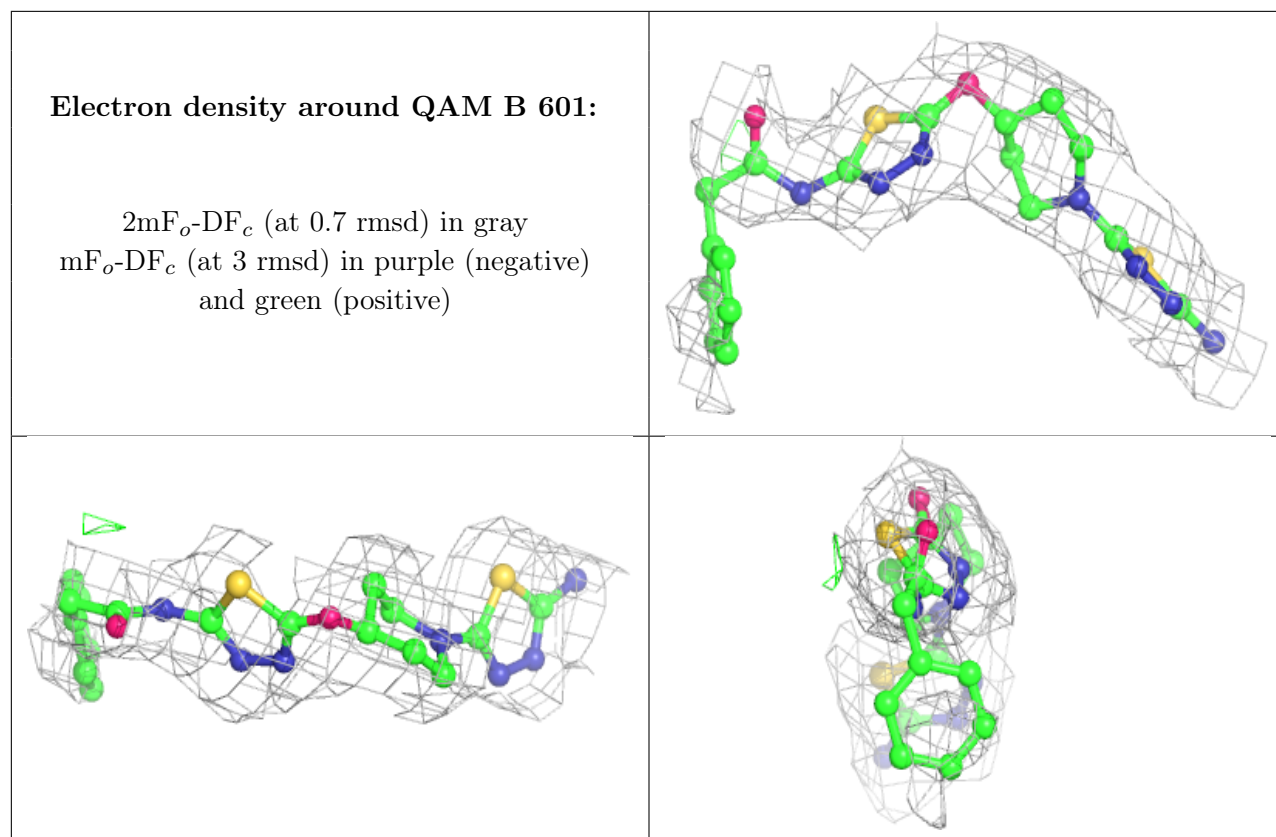
6.4 Ligands [i](#)

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, 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(Å ²)	Q<0.9
2	QAM	C	601	28/28	0.83	0.23	58,79,102,114	0
2	QAM	B	601	28/28	0.91	0.21	51,76,116,130	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.