



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:16 PM UTC

PDB ID : 6UMF / pdb_00006umf
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 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

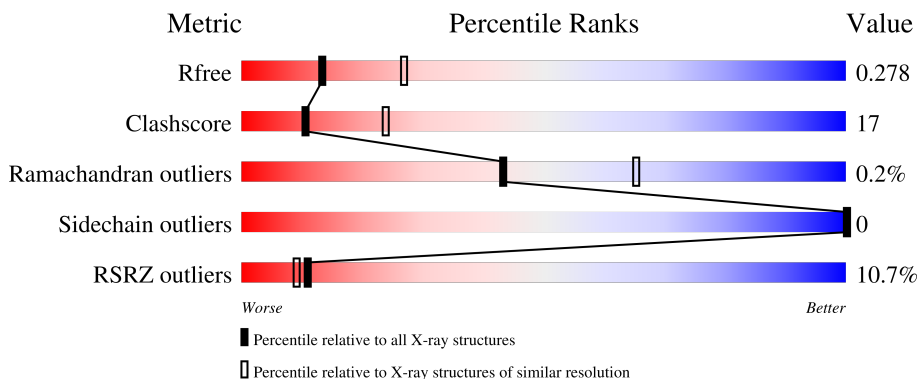
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (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 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	527	7% 53% 24% 22%
1	B	527	9% 54% 23% 22%
1	C	527	9% 55% 23% 22%
1	D	527	9% 50% 27% • 22%

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.

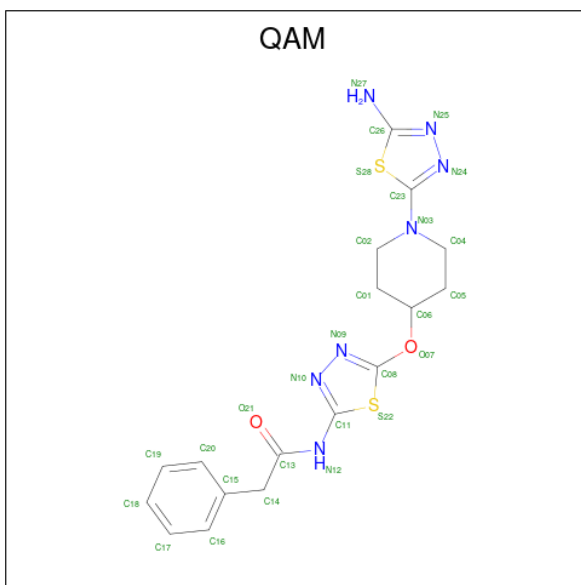
- Molecule 1 is a protein called Glutaminase kidney isoform, mitochondrial.

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 (CCD ID: QAM) (formula: C₁₇H₁₉N₇O₂S₂) (labeled as "Ligand of Interest" by depositor).



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

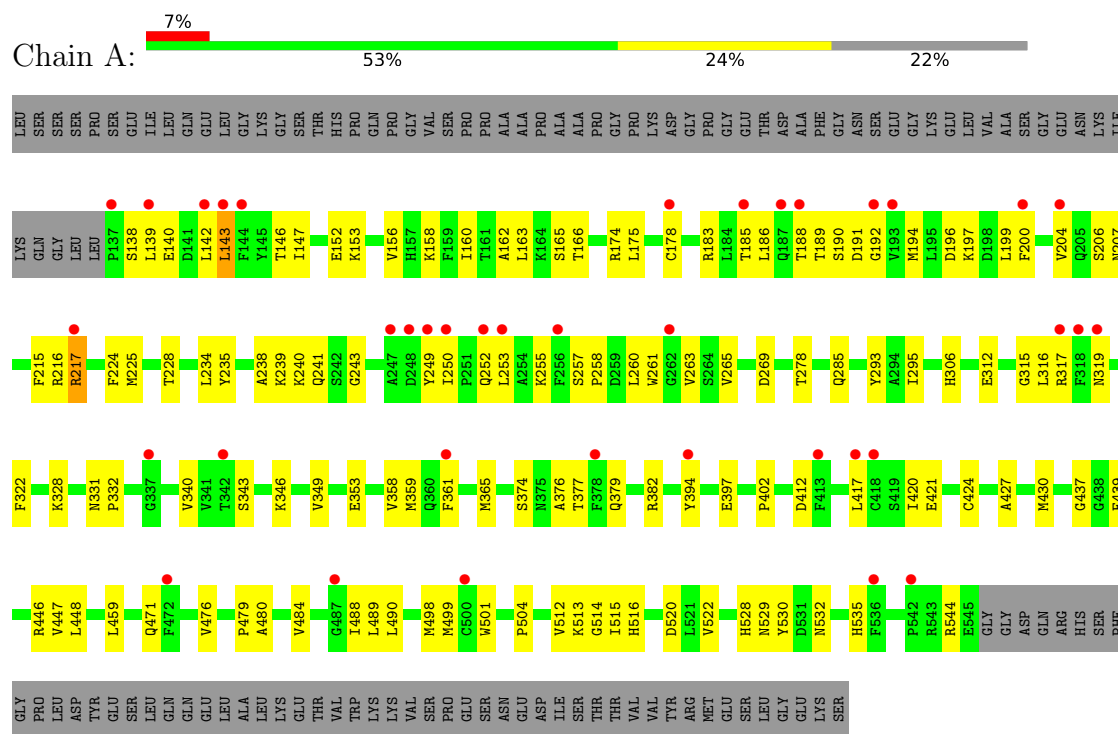
- Molecule 3 is water.

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

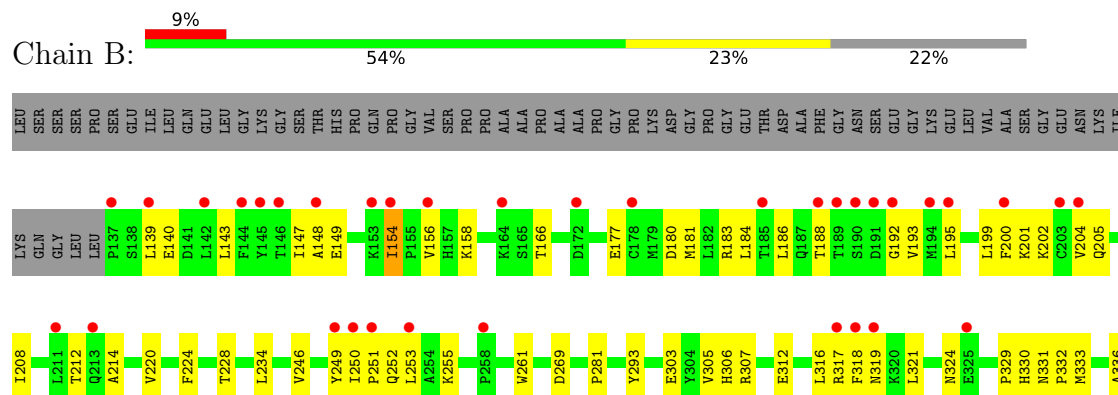
3 Residue-property plots [i](#)

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

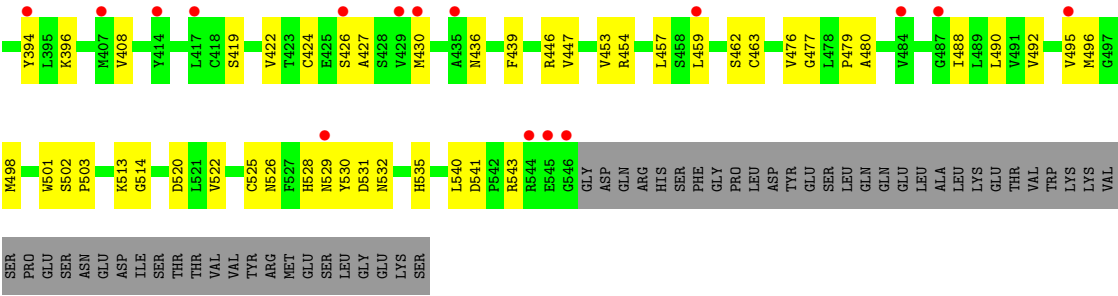
- Molecule 1: Glutaminase kidney isoform, mitochondrial



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.73Å 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 0.218 , 0.278	Depositor DCC
R_{free} test set	1984 reflections (2.95%)	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)	0.35 , 58.2	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

5.1 Standard geometry

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	0.43	0/3262	0.72	5/4403 (0.1%)
1	B	0.41	0/3266	0.73	2/4408 (0.0%)
1	C	0.46	0/3266	0.79	5/4408 (0.1%)
1	D	0.43	0/3266	0.77	8/4408 (0.2%)
All	All	0.43	0/13060	0.75	20/17627 (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

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	153	LYS	CA-CB-CG	9.46	133.02	114.10
1	C	152	GLU	CA-C-N	9.45	137.43	122.59
1	C	152	GLU	C-N-CA	9.45	137.43	122.59
1	B	544	ARG	CB-CG-CD	-7.61	93.79	111.30
1	D	143	LEU	CA-CB-CG	-7.16	91.23	116.30
1	D	152	GLU	CA-C-N	6.70	133.65	122.87
1	D	152	GLU	C-N-CA	6.70	133.65	122.87
1	C	245	LYS	CG-CD-CE	6.52	126.30	111.30
1	A	217	ARG	CA-CB-CG	-6.12	101.87	114.10
1	C	143	LEU	CD1-CG-CD2	6.08	124.18	110.80
1	A	143	LEU	CB-CG-CD2	-5.94	92.88	110.70
1	A	190	SER	CA-C-O	5.90	128.95	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	LYS	CG-CD-CE	5.83	124.70	111.30
1	D	152	GLU	CB-CA-C	-5.72	99.03	110.42
1	C	197	LYS	CB-CG-CD	-5.70	98.20	111.30
1	D	199	LEU	CB-CG-CD2	-5.69	93.63	110.70
1	D	153	LYS	CB-CG-CD	5.63	124.26	111.30
1	B	154	ILE	CA-CB-CG1	5.61	119.94	110.40
1	D	143	LEU	CB-CG-CD2	5.04	125.82	110.70
1	A	190	SER	O-C-N	5.01	129.25	122.59

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	110	0
1	B	3194	0	3170	105	0
1	C	3194	0	3170	104	0
1	D	3194	0	3170	129	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	429	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 17.

All (429) 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:B:490:LEU:HD23	1:B:498:MET:HE3	1.57	0.86
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:333:MET:N	1:D:333:MET:HE2	1.97	0.79
1:D:143:LEU:HD13	1:D:208:ILE:HD11	1.63	0.78
1:D:155:PRO:HG3	1:D:194:MET:HE3	1.65	0.78
1:D:166:THR:HG21	1:D:214:ALA:HB1	1.66	0.78
1:B:489:LEU:HD12	1:B:499:MET:HE2	1.65	0.78
1:D:265:VAL:HG22	1:D:498:MET:HE2	1.65	0.77
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:A:189:THR:C	1:A:191:ASP:H	1.96	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: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:HZ1	1:C:205:GLN:HG3	1.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:332:PRO:HB2	1:D:333:MET:HE1	1.80	0.64
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: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:A:265:VAL:HG22	1:A:498:MET:HE2	1.81	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:D:333:MET:HE3	1:D:459:LEU:HB3	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: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:D:177:GLU:CD	1:D:177:GLU:H	2.10	0.60
1:D:359:MET:HE1	1:D:371:VAL:HG23	1.83	0.60
1:A:143:LEU:CD2	1:A:200:PHE:HZ	2.14	0.59
1:A:544:ARG:HA	1:A:544:ARG:NH1	2.17	0.59
1:C:174:ARG:NH1	1:C:269:ASP:O	2.33	0.59
1:B:148:ALA:O	1:B:149:GLU:HB2	2.01	0.59
1:A:349:VAL:CG1	1:A:353:GLU:HB2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:GLN:HG2	3:D:618:HOH:O	2.02	0.59
1:B:333:MET:HE3	1:B:459:LEU:HB3	1.85	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:153:LYS:HB3	1:C:195:LEU:C	2.28	0.58
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:HD12	1:A:139:LEU:H	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:D:362:LEU:HD22	1:D:430:MET:HE1	1.87	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:D:170:THR:HB	1:D:179:MET:HE2	1.87	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:B:177:GLU:CD	1:B:177:GLU:H	2.15	0.55
1:C:178:CYS:SG	1:C:204:VAL:HG12	2.46	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:365:MET:HG3	1:C:447:VAL:HG11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:ALA:HB2	1:B:490:LEU:HD12	1.90	0.54
1:C:293:TYR:OH	1:C:306:HIS:NE2	2.35	0.54
1:D:365:MET:HG3	1:D:447:VAL:HG11	1.90	0.54
1:A:479:PRO:HG3	1:D:530:TYR:CE1	2.42	0.53
1:B:261:TRP:HA	1:B:501:TRP:O	2.07	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
1:A:138:SER:O	1:A:142:LEU:CD2	2.56	0.53
1:A:544:ARG:HA	1:A:544:ARG:HH11	1.73	0.53
1:B:140:GLU:CB	1:B:201:LYS:HG3	2.38	0.53
1:C:332:PRO:HB2	1:C:333:MET:HE2	1.91	0.53
1:C:480:ALA:HB2	1:C:490:LEU:HD12	1.90	0.53
1:A:315:GLY:C	1:A:317:ARG:H	2.16	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: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:283:CYS:HB3	1:C:419:SER:HA	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: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:D:492:VAL:HG21	1:D:496:MET:HE2	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:540:LEU:HD13	1:D:541:ASP:C	2.35	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
1:C:149:GLU:O	1:C:149:GLU:HG2	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: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:A:489:LEU:HD12	1:A:499:MET:HE2	1.92	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:252:GLN:NE2	1:A:376:ALA:O	2.45	0.49
1:A:374:SER:OG	1:A:377:THR:HG23	2.12	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: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:C:181:MET:HE3	1:C:202:LYS:HE2	1.93	0.49
1:C:322:PHE:C	1:C:323:LEU:HD23	2.38	0.49
1:D:350:ASN:HD22	1:D:352:ALA:N	2.06	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:143:LEU:HD12	1:C:208:ILE:HD11	1.95	0.49
1:C:153:LYS:HB3	1:C:195:LEU:O	2.12	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:153:LYS:HD3	1:C:194:MET:HE3	1.94	0.48
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:A:529:ASN:CG	1:D:529:ASN:HD21	2.21	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:C:316:LEU:HD21	1:C:467:ASP:HB3	1.96	0.48
1:A:315:GLY:C	1:A:317:ARG:N	2.72	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: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: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:489:LEU:HD12	1:C:499:MET:HE2	1.96	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:153:LYS:CD	1:A:196:ASP:HB3	2.44	0.47
1:A:239:LYS:HG2	1:A:239:LYS:O	2.14	0.47
1:A:315:GLY:O	1:A:317:ARG:N	2.48	0.47
1:A:317:ARG:HD3	2:C:601:QAM:C19	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:153:LYS:CD	1:C:194:MET:HE3	2.45	0.47
1:B:261:TRP:HZ3	1:B:500:CYS:HB3	1.80	0.46
1:B:319:ASN:OD1	1:B:319:ASN:N	2.48	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
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:B:140:GLU:HG3	1:B:208:ILE:HG12	1.97	0.46
1:B:181:MET:HE2	1:B:202:LYS:HG2	1.96	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:B:492:VAL:HG21	1:B:496:MET:HE2	1.97	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:264:SER:HB3	1:D:424:CYS:HB3	1.98	0.46
1:D:286:SER:O	1:D:289:LYS:HG3	2.16	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:C:179:MET:HE3	1:C:179:MET:HB3	1.67	0.45
1:D:260:LEU:HD13	1:D:501:TRP:CH2	2.51	0.45
1:C:140:GLU:OE1	1:C:140:GLU:N	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:N	1:B:455:ASN:HD22	2.14	0.45
1:B:507:LYS:HD3	1:B:507:LYS:HA	1.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:320:LYS:HZ3	2:C:601:QAM:C16	2.29	0.45
1:B:312:GLU:O	1:B:331:ASN:ND2	2.47	0.45
1:C:315:GLY:C	1:C:317:ARG:H	2.24	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
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:498:MET:HE2	1:B:498:MET:HB2	1.84	0.44
1:C:372:GLY:C	1:C:421:GLU:H	2.25	0.44
1:C:407:MET:SD	1:C:407:MET:C	3.00	0.44
1:B:544:ARG:HA	1:B:544:ARG:HD2	1.42	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:153:LYS:HB2	1:A:194:MET:SD	2.58	0.44
1:A:185:THR:HA	1:A:188:THR:OG1	2.18	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: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:293:TYR:OH	1:D:306:HIS:NE2	2.33	0.44
1:D:308:TYR:HB3	1:D:340:VAL:HG11	1.99	0.44
1:D:332:PRO:HB2	1:D:333:MET:CE	2.46	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:304:TYR:CD2	1:D:304:TYR:C	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:315:GLY:C	1:C:317:ARG:N	2.76	0.43
1:C:526:ASN:HD21	1:C:541:ASP:CG	2.25	0.43
1:B:490:LEU:CD2	1:B:498:MET:HE3	2.38	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:D:332:PRO:C	1:D:333:MET:HE2	2.43	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:C:154:ILE:C	1:C:194:MET:HG3	2.44	0.43
1:B:293:TYR:HE1	1:B:305:VAL:HG11	1.84	0.43
1:C:231:ILE:HD13	1:C:231:ILE:HA	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:HG23	1:A:189:THR:O	2.19	0.43
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:286:SER:HB3	1:D:289:LYS:HZ3	1.83	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:149:GLU:C	1:D:151:GLN:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:206:SER:C	1:A:207:ASN:HD22	2.28	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: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:D:148:ALA:HA	1:D:154:ILE:CG2	2.49	0.41
1:A:293:TYR:OH	1:A:306:HIS:NE2	2.37	0.41
1:D:261:TRP:CD1	1:D:513:LYS:HD2	2.55	0.41
1:D:324:ASN:OD1	1:D:324:ASN:C	2.63	0.41
1:C:255:LYS:O	1:C:255:LYS:HG2	2.20	0.41
1:C:261:TRP:HA	1:C:501:TRP:O	2.19	0.41
1:C:349:VAL:O	1:C:354:LYS:HE3	2.20	0.41
1:D:274:SER:HB3	1:D:278:THR:HG21	2.03	0.41
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:B:489:LEU:CD1	1:B:499:MET:HE2	2.43	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:B:467:ASP:HB2	1:B:508:MET:HE2	2.03	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:A:197:LYS:HE3	1:A:197:LYS:HB3	1.85	0.41
1:A:243:GLY:O	1:A:512:VAL:HG21	2.21	0.41
1:B:166:THR:CG2	1:B:214:ALA:HB1	2.45	0.41
1:B:184:LEU:O	1:B:188:THR:HG23	2.20	0.41
1:D:522:VAL:CG1	1:D:528:HIS:HB2	2.51	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:HD23	1:B:316:LEU:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:165:SER:O	1:A:225:MET:HE3	2.22	0.40
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:HA	1:A:316:LEU:HD23	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:HE3	1:A:255:LYS:HB3	1.95	0.40
1:B:525:CYS:HA	1:B:540:LEU:O	2.22	0.40
1:C:293:TYR:HH	1:C:306:HIS:HE2	1.60	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%)	43	65
1	B	408/527 (77%)	393 (96%)	14 (3%)	1 (0%)	43	65
1	C	408/527 (77%)	395 (97%)	12 (3%)	1 (0%)	43	65
1	D	408/527 (77%)	391 (96%)	16 (4%)	1 (0%)	43	65
All	All	1631/2108 (77%)	1575 (97%)	52 (3%)	4 (0%)	43	65

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%)	353 (100%)	0	100	100
1	B	353/451 (78%)	353 (100%)	0	100	100
1	C	353/451 (78%)	353 (100%)	0	100	100
1	D	353/451 (78%)	353 (100%)	0	100	100
All	All	1412/1804 (78%)	1412 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	207	ASN
1	A	368	ASN
1	A	416	GLN
1	A	455	ASN
1	A	471	GLN
1	A	516	HIS
1	A	519	HIS
1	B	187	GLN
1	B	230	HIS
1	B	330	HIS
1	B	360	GLN
1	B	510	ASN
1	C	285	GLN
1	C	388	ASN
1	C	416	GLN

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Mol	Chain	Res	Type
1	C	455	ASN
1	C	519	HIS
1	C	535	HIS
1	D	330	HIS
1	D	350	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	31,31,31	2.52	10 (32%)	41,42,42	6.24	20 (48%)
2	QAM	C	601	-	31,31,31	2.49	8 (25%)	41,42,42	4.34	21 (51%)

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	-	-	8/14/26/26	0/4/4/4
2	QAM	C	601	-	-	8/14/26/26	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	QAM	C26-N27	6.04	1.46	1.34
2	C	601	QAM	C26-N27	5.63	1.45	1.34
2	B	601	QAM	C13-N12	5.38	1.47	1.37
2	C	601	QAM	C13-N12	5.27	1.46	1.37
2	C	601	QAM	C11-N12	5.25	1.46	1.38
2	B	601	QAM	C11-N12	5.04	1.45	1.38
2	C	601	QAM	C23-N03	4.49	1.44	1.34
2	C	601	QAM	C02-N03	4.49	1.55	1.47
2	B	601	QAM	C04-N03	4.39	1.54	1.47
2	B	601	QAM	C23-N03	4.24	1.44	1.34
2	B	601	QAM	C02-N03	4.21	1.54	1.47
2	B	601	QAM	C08-N09	3.86	1.33	1.29
2	C	601	QAM	C04-N03	3.81	1.53	1.47
2	C	601	QAM	C08-N09	3.61	1.33	1.29
2	C	601	QAM	O07-C08	3.35	1.40	1.35
2	B	601	QAM	O07-C08	2.98	1.39	1.35
2	B	601	QAM	C01-C06	-2.34	1.44	1.51
2	B	601	QAM	C08-S22	-2.10	1.71	1.75

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	QAM	C06-O07-C08	-29.69	98.19	117.71
2	C	601	QAM	C06-O07-C08	-11.11	110.41	117.71
2	B	601	QAM	S28-C26-N25	-10.44	106.31	113.79
2	C	601	QAM	S28-C26-N25	-10.02	106.61	113.79
2	B	601	QAM	C26-S28-C23	9.97	94.94	86.42
2	C	601	QAM	C26-S28-C23	9.68	94.69	86.42
2	B	601	QAM	C08-N09-N10	9.60	116.90	105.84
2	C	601	QAM	C08-N09-N10	9.40	116.67	105.84
2	C	601	QAM	S22-C08-N09	-8.27	106.34	117.59
2	B	601	QAM	S22-C08-N09	-8.04	106.65	117.59
2	C	601	QAM	S22-C11-N10	-6.90	106.81	114.52
2	B	601	QAM	C02-C01-C06	-6.78	102.98	110.32
2	B	601	QAM	N12-C11-N10	6.22	126.37	120.81
2	B	601	QAM	S22-C11-N10	-6.12	107.69	114.52
2	B	601	QAM	N03-C23-N24	5.94	128.39	116.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	QAM	N12-C11-N10	5.50	125.72	120.81
2	B	601	QAM	O07-C08-S22	5.15	127.25	116.13
2	C	601	QAM	N03-C23-N24	4.95	126.48	116.91
2	C	601	QAM	S28-C23-N03	4.72	126.63	120.31
2	C	601	QAM	C14-C13-N12	4.65	120.07	114.40
2	C	601	QAM	C23-N24-N25	4.57	116.10	107.08
2	B	601	QAM	C23-N24-N25	4.49	115.93	107.08
2	C	601	QAM	S28-C23-N24	-4.36	106.89	114.44
2	B	601	QAM	S28-C23-N24	-4.27	107.05	114.44
2	C	601	QAM	O07-C08-S22	4.15	125.08	116.13
2	C	601	QAM	C11-S22-C08	4.05	95.00	86.65
2	B	601	QAM	S28-C26-N27	4.00	127.19	121.97
2	B	601	QAM	C26-N25-N24	3.96	115.75	112.07
2	C	601	QAM	C26-N25-N24	3.92	115.71	112.07
2	B	601	QAM	O07-C06-C05	3.89	117.56	108.37
2	B	601	QAM	C11-S22-C08	3.80	94.47	86.65
2	C	601	QAM	S28-C26-N27	3.70	126.79	121.97
2	B	601	QAM	C14-C13-N12	3.35	118.49	114.40
2	C	601	QAM	N27-C26-N25	3.29	126.60	123.83
2	B	601	QAM	N27-C26-N25	3.18	126.50	123.83
2	B	601	QAM	S28-C23-N03	3.12	124.49	120.31
2	C	601	QAM	S22-C11-N12	2.79	127.45	123.72
2	C	601	QAM	C11-N10-N09	2.48	115.17	112.02
2	C	601	QAM	C04-C05-C06	-2.19	107.95	110.32
2	C	601	QAM	C05-C06-C01	-2.10	107.39	111.67
2	B	601	QAM	C04-C05-C06	-2.01	108.15	110.32

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	QAM	S22-C11-N12-C13
2	B	601	QAM	N24-C23-N03-C02
2	B	601	QAM	N24-C23-N03-C04
2	B	601	QAM	S28-C23-N03-C02
2	B	601	QAM	S28-C23-N03-C04
2	C	601	QAM	N10-C11-N12-C13
2	C	601	QAM	S22-C11-N12-C13
2	C	601	QAM	N24-C23-N03-C04
2	B	601	QAM	N10-C11-N12-C13
2	B	601	QAM	O21-C13-C14-C15
2	C	601	QAM	S28-C23-N03-C02

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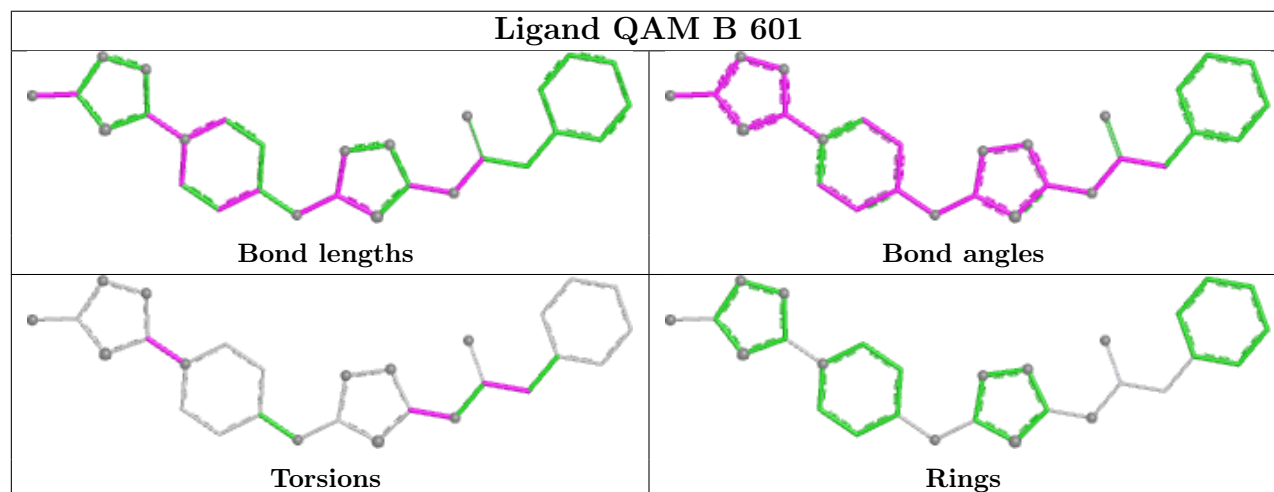
Mol	Chain	Res	Type	Atoms
2	C	601	QAM	S28-C23-N03-C04
2	C	601	QAM	O21-C13-C14-C15
2	B	601	QAM	N12-C13-C14-C15
2	C	601	QAM	N12-C13-C14-C15
2	C	601	QAM	N24-C23-N03-C02

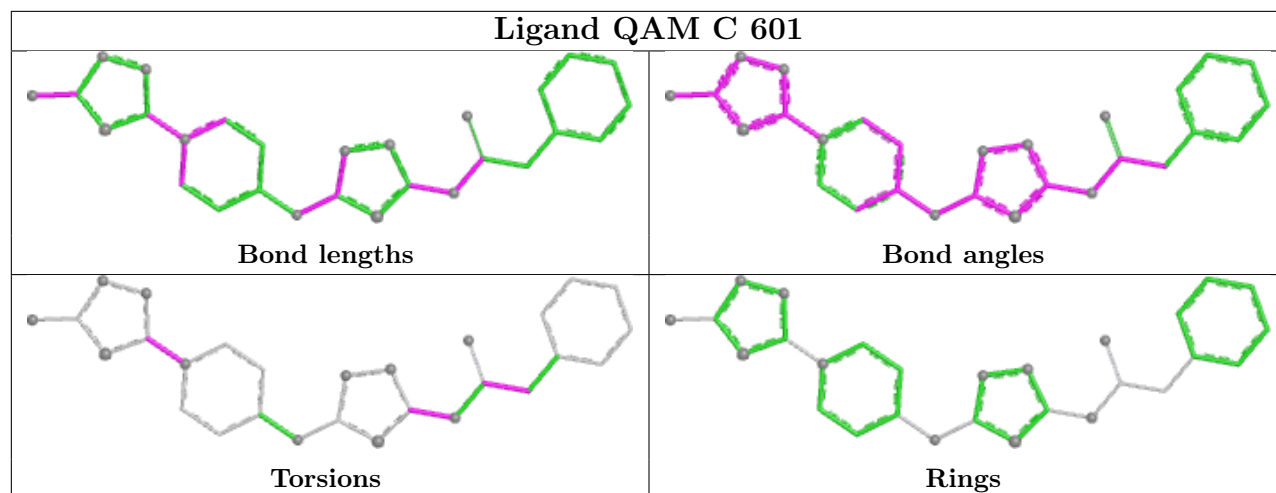
There are no ring outliers.

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%)	0.84	38 (9%) 14 12	31, 52, 96, 157	0
1	B	410/527 (77%)	0.92	47 (11%) 9 8	30, 51, 102, 169	0
1	C	410/527 (77%)	0.90	45 (10%) 10 8	26, 48, 97, 137	0
1	D	410/527 (77%)	0.83	46 (11%) 10 8	25, 49, 94, 164	0
All	All	1639/2108 (77%)	0.87	176 (10%) 11 9	25, 50, 97, 169	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	144	PHE	6.3
1	C	144	PHE	5.4
1	B	200	PHE	5.4
1	C	546	GLY	5.3
1	D	318	PHE	5.0
1	B	189	THR	5.0
1	D	189	THR	4.8
1	D	546	GLY	4.7
1	B	253	LEU	4.6
1	D	193	VAL	4.6
1	C	318	PHE	4.5
1	A	192	GLY	4.5
1	D	200	PHE	4.5
1	B	191	ASP	4.4
1	B	318	PHE	4.4
1	B	153	LYS	4.3
1	A	318	PHE	4.3
1	B	185	THR	4.3
1	A	193	VAL	4.3
1	A	256	PHE	4.2
1	D	137	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	546	GLY	4.2
1	B	213	GLN	4.1
1	B	192	GLY	4.0
1	B	411	LEU	4.0
1	B	145	TYR	4.0
1	C	143	LEU	4.0
1	C	188	THR	3.9
1	B	144	PHE	3.9
1	A	249	TYR	3.9
1	C	193	VAL	3.9
1	B	172	ASP	3.9
1	C	200	PHE	3.7
1	C	249	TYR	3.7
1	B	137	PRO	3.6
1	B	190	SER	3.6
1	B	146	THR	3.5
1	C	342	THR	3.4
1	B	258	PRO	3.4
1	A	217	ARG	3.4
1	B	414	TYR	3.3
1	C	190	SER	3.3
1	B	250	ILE	3.3
1	B	251	PRO	3.3
1	D	316	LEU	3.3
1	C	189	THR	3.3
1	D	144	PHE	3.3
1	C	412	ASP	3.2
1	D	213	GLN	3.2
1	D	190	SER	3.2
1	D	366	ALA	3.1
1	B	188	THR	3.1
1	D	188	THR	3.0
1	D	407	MET	3.0
1	D	191	ASP	3.0
1	B	337	GLY	3.0
1	A	143	LEU	2.9
1	A	188	THR	2.9
1	D	319	ASN	2.9
1	A	204	VAL	2.9
1	D	417	LEU	2.9
1	C	154	ILE	2.9
1	C	214	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	143	LEU	2.9
1	D	153	LYS	2.8
1	A	139	LEU	2.8
1	D	148	ALA	2.8
1	C	195	LEU	2.8
1	D	142	LEU	2.8
1	C	319	ASN	2.8
1	D	211	LEU	2.8
1	A	253	LEU	2.7
1	B	142	LEU	2.7
1	D	430	MET	2.7
1	C	204	VAL	2.7
1	D	334	VAL	2.7
1	A	200	PHE	2.7
1	B	178	CYS	2.7
1	A	142	LEU	2.7
1	B	164	LYS	2.7
1	C	142	LEU	2.7
1	D	195	LEU	2.7
1	B	156	VAL	2.6
1	D	199	LEU	2.6
1	A	361	PHE	2.6
1	A	342	THR	2.6
1	A	250	ILE	2.6
1	B	417	LEU	2.6
1	C	317	ARG	2.6
1	D	414	TYR	2.6
1	A	542	PRO	2.6
1	B	317	ARG	2.5
1	D	164	LYS	2.5
1	C	397	GLU	2.5
1	A	262	GLY	2.5
1	D	372	GLY	2.5
1	C	137	PRO	2.5
1	D	145	TYR	2.5
1	A	472	PHE	2.5
1	C	498	MET	2.5
1	D	495	VAL	2.5
1	A	417	LEU	2.5
1	C	207	ASN	2.4
1	A	487	GLY	2.4
1	B	348	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	394	TYR	2.4
1	C	334	VAL	2.4
1	C	492	VAL	2.4
1	B	249	TYR	2.4
1	B	194	MET	2.4
1	C	139	LEU	2.3
1	A	248	ASP	2.3
1	C	511	SER	2.3
1	A	137	PRO	2.3
1	B	139	LEU	2.3
1	B	407	MET	2.3
1	B	445	GLU	2.3
1	A	500	CYS	2.3
1	C	220	VAL	2.3
1	A	252	GLN	2.3
1	A	178	CYS	2.3
1	B	319	ASN	2.3
1	D	429	VAL	2.3
1	A	247	ALA	2.2
1	D	225	MET	2.2
1	D	394	TYR	2.2
1	D	529	ASN	2.2
1	A	187	GLN	2.2
1	B	502	SER	2.2
1	D	172	ASP	2.2
1	C	487	GLY	2.2
1	D	487	GLY	2.2
1	B	204	VAL	2.2
1	C	316	LEU	2.2
1	A	536	PHE	2.2
1	C	336	ALA	2.2
1	B	500	CYS	2.2
1	D	544	ARG	2.2
1	B	211	LEU	2.2
1	A	378	PHE	2.2
1	B	338	ALA	2.2
1	B	154	ILE	2.2
1	B	148	ALA	2.2
1	C	431	ALA	2.2
1	D	342	THR	2.2
1	D	459	LEU	2.2
1	C	141	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	371	VAL	2.2
1	D	435	ALA	2.1
1	C	152	GLU	2.1
1	C	185	THR	2.1
1	D	185	THR	2.1
1	C	542	PRO	2.1
1	C	281	PRO	2.1
1	A	418	CYS	2.1
1	B	365	MET	2.1
1	D	545	GLU	2.1
1	B	195	LEU	2.1
1	B	203	CYS	2.1
1	C	308	TYR	2.1
1	A	413	PHE	2.1
1	B	325	GLU	2.1
1	A	185	THR	2.1
1	A	319	ASN	2.1
1	A	337	GLY	2.1
1	C	424	CYS	2.1
1	C	150	GLY	2.0
1	C	495	VAL	2.0
1	D	484	VAL	2.0
1	C	256	PHE	2.0
1	C	536	PHE	2.0
1	D	426	SER	2.0
1	C	252	GLN	2.0
1	D	192	GLY	2.0
1	A	317	ARG	2.0
1	D	156	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

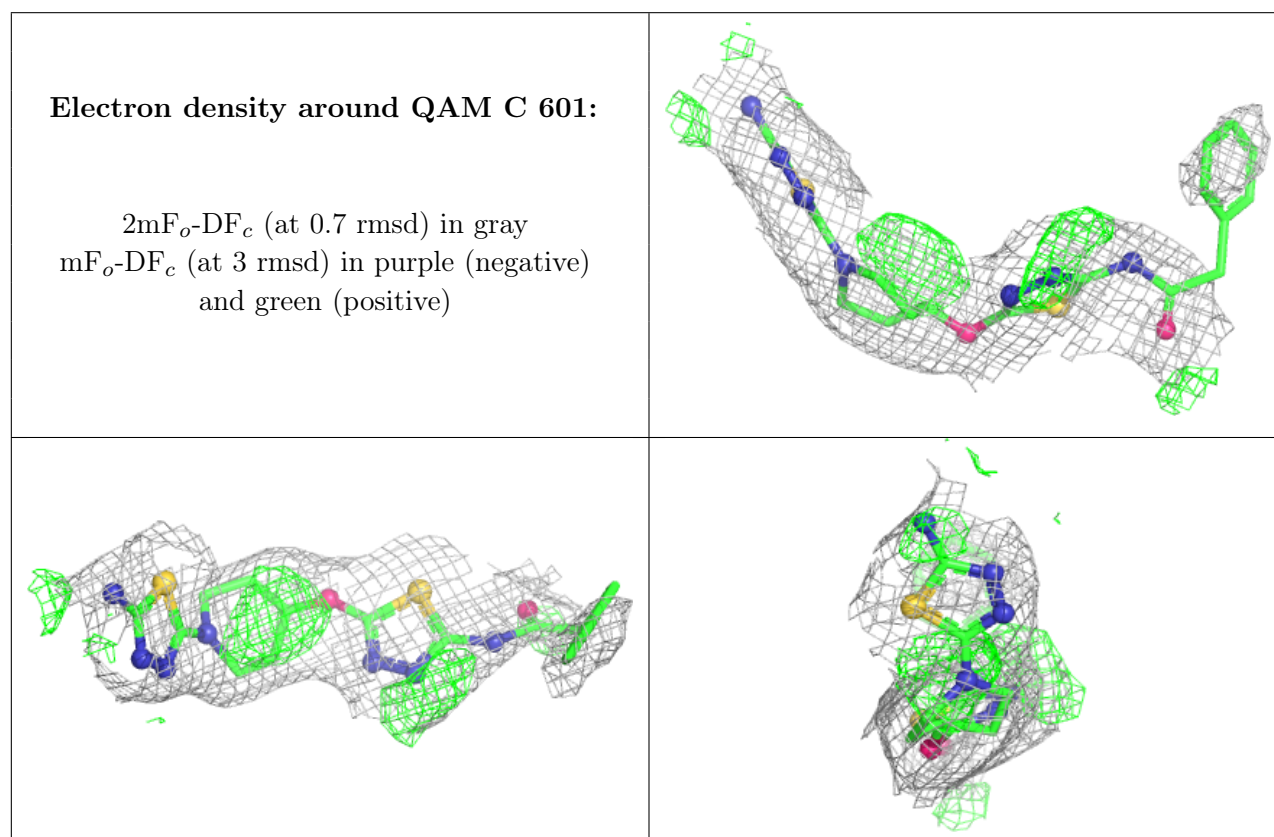
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

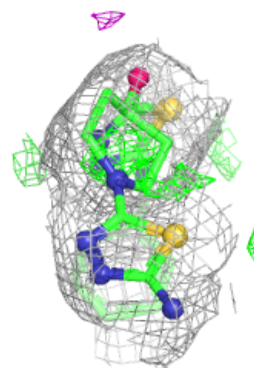
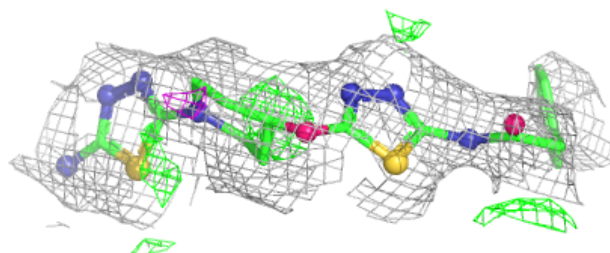
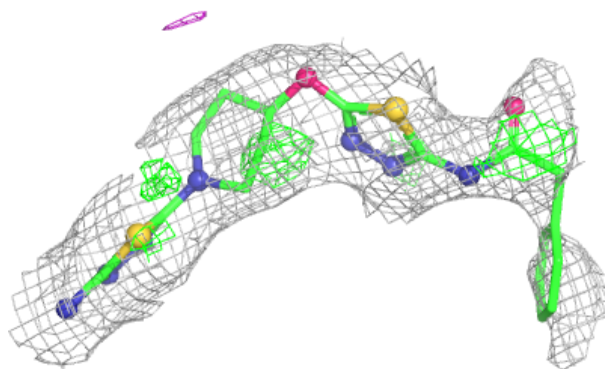
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	QAM	C	601	28/28	0.87	0.18	58,79,102,114	0
2	QAM	B	601	28/28	0.91	0.16	51,76,116,130	0

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.



Electron density around QAM 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.