



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:45 PM UTC

PDB ID : 6UMD / pdb_00006umd
Title : Crystal structure of human GAC in complex with inhibitor UPGL00012
Authors : Huang, Q.; Cerione, R.A.
Deposited on : 2019-10-09
Resolution : 2.70 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

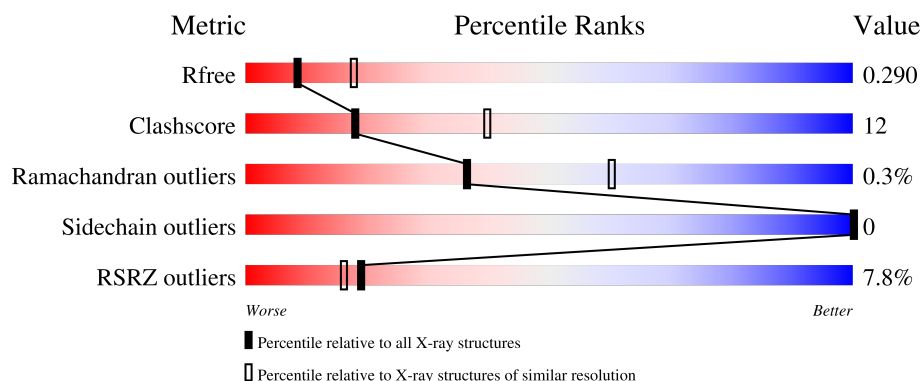
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	6% 57% 18% • 24%
1	B	527	6% 57% 19% • 22%
1	C	527	8% 57% 20% • 22%
1	D	527	5% 59% 18% • 22%

2 Entry composition [i](#)

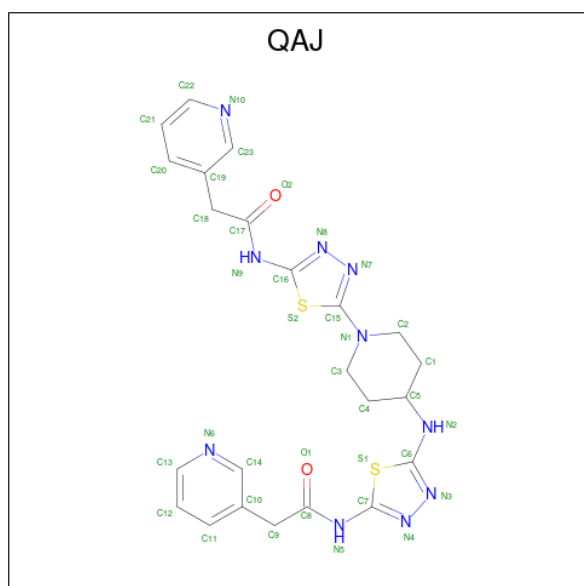
There are 3 unique types of molecules in this entry. The entry contains 12842 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	403	Total	C	N	O	S	1	0	0
			3146	2005	531	582	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-(pyridin-3-yl)-N-(5-{4-[(5-{[(pyridin-3-yl)acetyl]amino}-1,3,4-thiadiazol-2-yl)amino]piperidin-1-yl}-1,3,4-thiadiazol-2-yl)acetamide (CCD ID: QAJ) (formula: C₂₃H₂₄N₁₀O₂S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			37	23	10	2	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	S	0	0
			37	23	10	2	2		

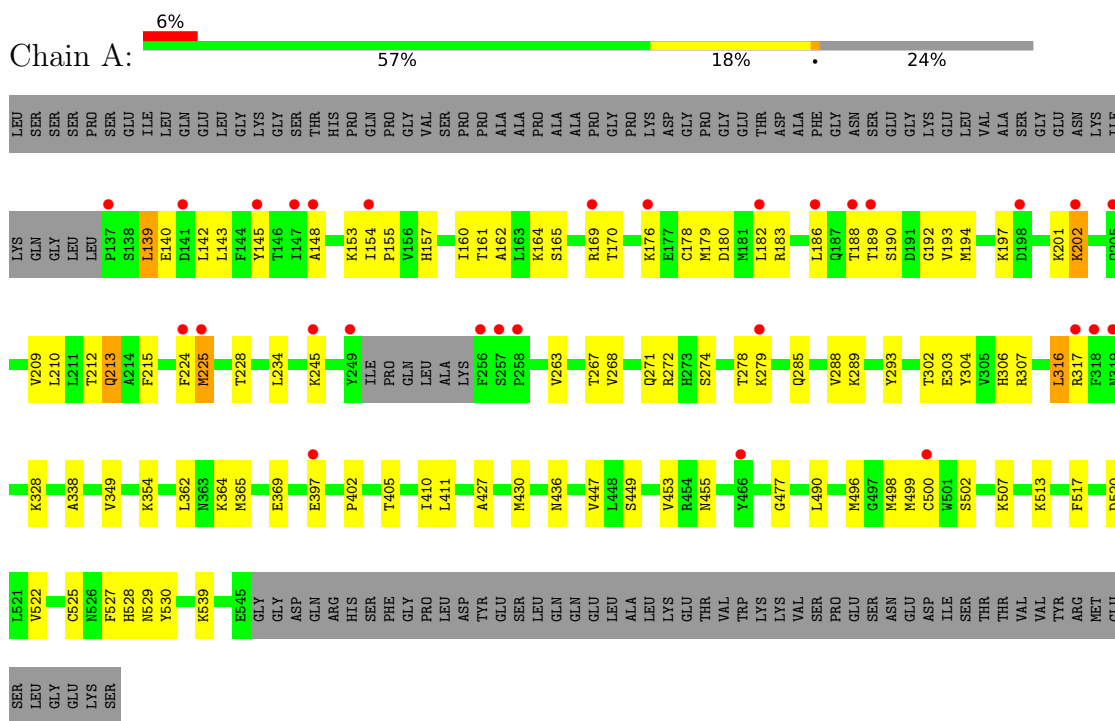
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	10	Total	O	0	0
			10	10		
3	C	11	Total	O	0	0
			11	11		
3	D	14	Total	O	0	0
			14	14		

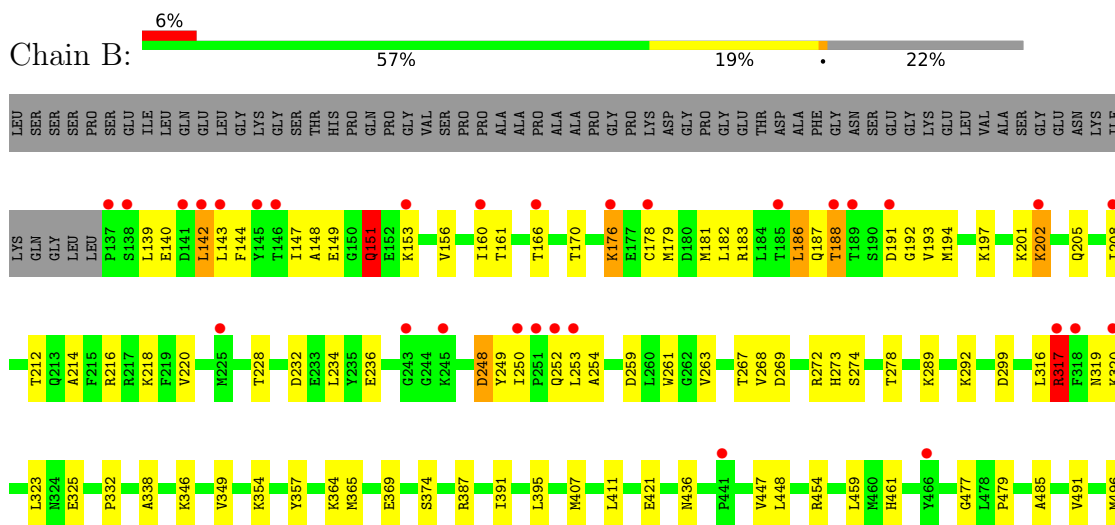
3 Residue-property plots [i](#)

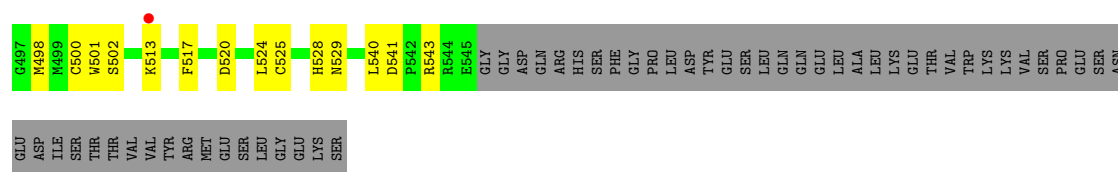
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

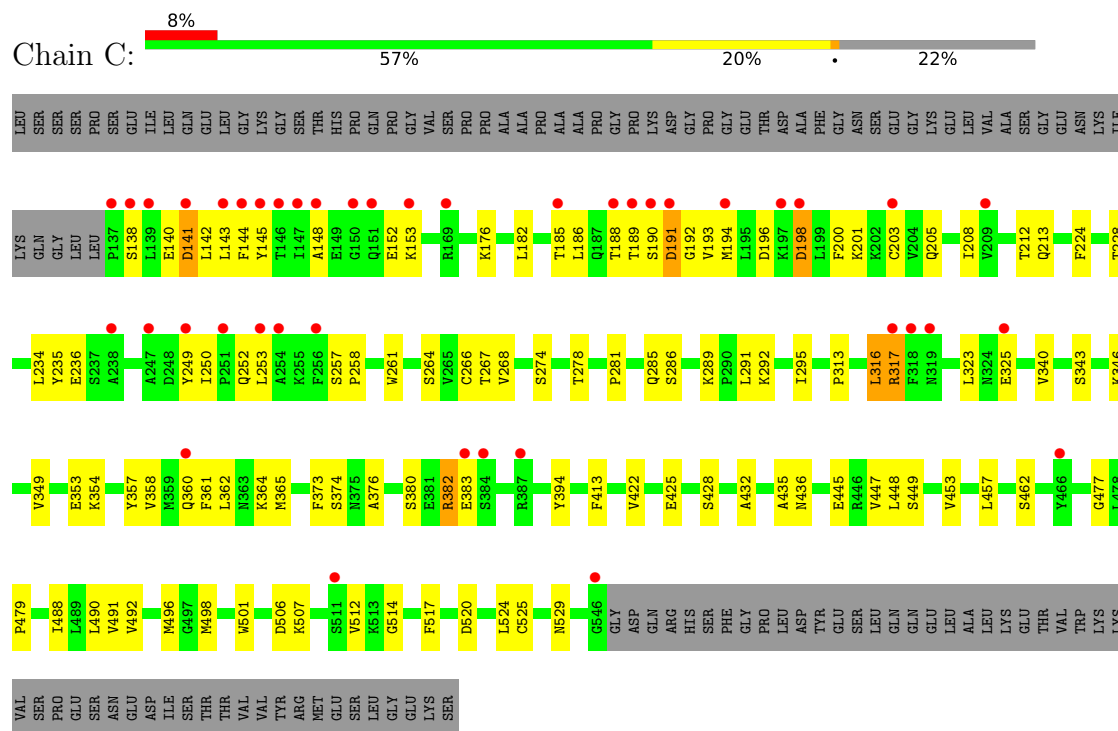


- Molecule 1: Glutaminase kidney isoform, mitochondrial

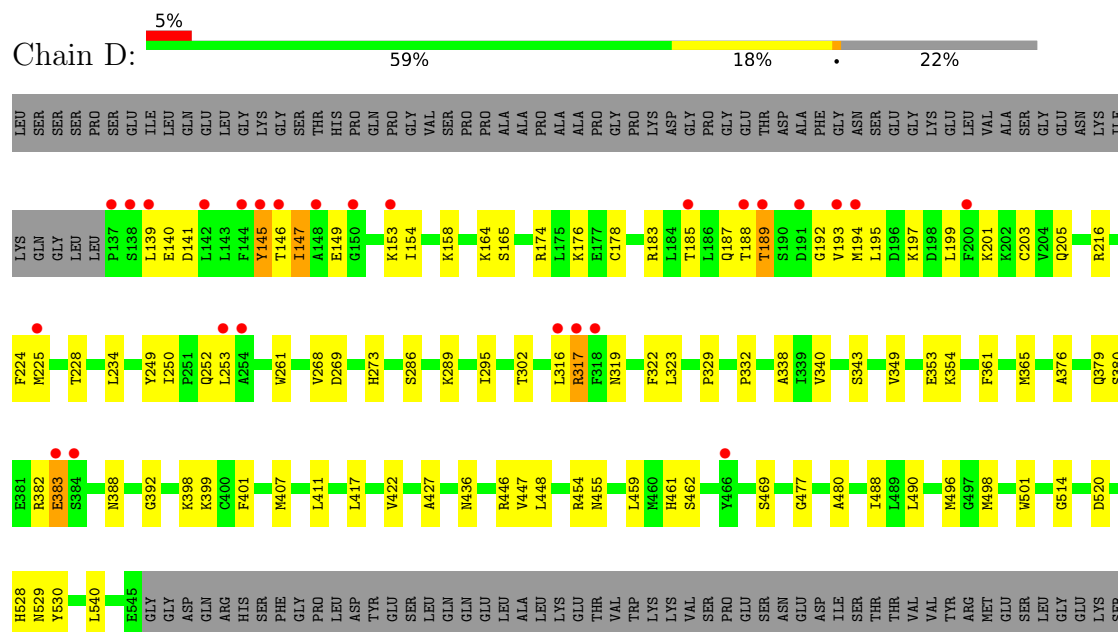




- Molecule 1: Glutaminase kidney isoform, mitochondrial



- 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, α , β , γ	100.48Å 139.16Å 178.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.23 – 2.70 20.23 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.23-2.70) 98.3 (20.23-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.71Å)	Xtrriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.228 , 0.288 0.228 , 0.290	Depositor DCC
R_{free} test set	2000 reflections (2.32%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtrriage
Anisotropy	1.162	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12842	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.47 % 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 2.3565e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: QAJ

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	0.55	0/3216	0.90	13/4339 (0.3%)
1	B	0.52	0/3264	0.90	11/4406 (0.2%)
1	C	0.55	1/3268 (0.0%)	0.94	15/4411 (0.3%)
1	D	0.51	0/3264	0.88	13/4406 (0.3%)
All	All	0.53	1/13012 (0.0%)	0.91	52/17562 (0.3%)

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	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	191	ASP	CA-CB	8.97	1.68	1.53

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	382	ARG	CA-C-N	-11.92	104.02	122.37
1	C	382	ARG	C-N-CA	-11.92	104.02	122.37
1	B	142	LEU	CB-CA-C	-10.36	90.77	110.67
1	B	186	LEU	CA-CB-CG	9.54	149.69	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	382	ARG	CA-C-N	9.11	138.39	122.09
1	D	382	ARG	C-N-CA	9.11	138.39	122.09
1	D	383	GLU	N-CA-CB	-8.94	97.42	110.47
1	C	325	GLU	CA-CB-CG	-8.62	96.86	114.10
1	A	411	LEU	CB-CG-CD2	-8.61	84.87	110.70
1	B	248	ASP	CB-CA-C	-8.38	95.45	109.03
1	D	398	LYS	CD-CE-NZ	-8.16	85.78	111.90
1	C	190	SER	CA-C-N	-7.85	111.27	123.13
1	C	190	SER	C-N-CA	-7.85	111.27	123.13
1	C	198	ASP	CB-CA-C	7.49	124.11	109.72
1	D	399	LYS	CB-CG-CD	-7.29	94.53	111.30
1	D	383	GLU	CA-CB-CG	7.25	128.59	114.10
1	C	176	LYS	CD-CE-NZ	7.17	134.84	111.90
1	C	383	GLU	CB-CG-CD	-7.12	100.50	112.60
1	C	317	ARG	CG-CD-NE	-7.01	96.58	112.00
1	D	398	LYS	CG-CD-CE	7.00	127.40	111.30
1	B	142	LEU	N-CA-CB	6.99	121.11	110.28
1	A	225	MET	CB-CG-SD	-6.70	92.61	112.70
1	B	176	LYS	CA-CB-CG	-6.60	100.89	114.10
1	B	151	GLN	CA-CB-CG	6.57	127.24	114.10
1	A	202	LYS	CD-CE-NZ	-6.20	92.05	111.90
1	D	149	GLU	CA-CB-CG	5.89	125.88	114.10
1	D	147	ILE	CG1-CB-CG2	-5.87	93.11	110.70
1	A	176	LYS	CB-CG-CD	5.83	124.70	111.30
1	C	213	GLN	CB-CA-C	5.80	121.36	110.63
1	D	189	THR	CA-C-N	5.76	132.01	122.73
1	D	189	THR	C-N-CA	5.76	132.01	122.73
1	B	191	ASP	N-CA-C	5.73	120.07	111.81
1	D	398	LYS	CB-CG-CD	-5.73	98.11	111.30
1	C	360	GLN	CA-CB-CG	5.64	125.37	114.10
1	A	279	LYS	CG-CD-CE	5.63	124.24	111.30
1	B	248	ASP	N-CA-CB	5.57	118.00	110.59
1	A	139	LEU	CA-CB-CG	5.53	135.65	116.30
1	B	202	LYS	CG-CD-CE	-5.53	98.59	111.30
1	B	317	ARG	CD-NE-CZ	-5.48	116.73	124.40
1	A	213	GLN	N-CA-CB	-5.42	101.33	110.49
1	C	198	ASP	N-CA-CB	-5.37	102.03	110.46
1	A	303	GLU	CA-CB-CG	5.34	124.78	114.10
1	A	176	LYS	CD-CE-NZ	5.31	128.89	111.90
1	A	303	GLU	CB-CA-C	5.28	120.27	109.55
1	A	279	LYS	CB-CG-CD	-5.22	99.29	111.30
1	A	202	LYS	CB-CG-CD	5.22	123.30	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	317	ARG	N-CA-C	-5.17	99.79	110.80
1	C	383	GLU	CA-CB-CG	5.16	124.43	114.10
1	C	152	GLU	CA-CB-CG	5.16	124.42	114.10
1	A	397	GLU	CB-CG-CD	-5.13	103.88	112.60
1	C	176	LYS	CB-CG-CD	5.11	123.05	111.30
1	D	383	GLU	CB-CG-CD	5.11	121.28	112.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	316	LEU	Peptide
1	A	317	ARG	Peptide
1	B	316	LEU	Peptide
1	B	317	ARG	Peptide
1	C	316	LEU	Peptide
1	C	317	ARG	Peptide
1	D	316	LEU	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	3146	0	3115	70	1
1	B	3192	0	3171	84	1
1	C	3196	0	3174	81	0
1	D	3192	0	3171	83	0
2	B	37	0	0	0	0
2	D	37	0	0	0	0
3	A	7	0	0	2	0
3	B	10	0	0	1	0
3	C	11	0	0	2	0
3	D	14	0	0	1	0
All	All	12842	0	12631	311	1

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 12.

All (311) 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:541:ASP:OD1	1:B:543:ARG:NH1	1.70	1.23
1:B:143:LEU:HD11	1:B:212:THR:HG22	1.31	1.08
1:D:141:ASP:OD1	1:D:197:LYS:HE3	1.55	1.05
1:D:407:MET:CE	1:D:411:LEU:HD23	1.87	1.04
1:B:216:ARG:HG2	1:B:218:LYS:HE3	1.49	0.93
1:D:141:ASP:CG	1:D:197:LYS:HE3	1.97	0.90
1:D:343:SER:HG	1:D:401:PHE:HD1	0.92	0.89
1:B:202:LYS:NZ	1:C:373:PHE:O	2.05	0.89
1:D:407:MET:HE3	1:D:411:LEU:HD23	1.53	0.89
1:D:407:MET:HE2	1:D:411:LEU:HD23	1.55	0.88
1:C:186:LEU:HD13	1:C:186:LEU:O	1.74	0.88
1:A:145:TYR:OH	1:A:197:LYS:NZ	2.08	0.86
1:A:210:LEU:HD12	1:A:213:GLN:HE21	1.39	0.84
1:B:139:LEU:HD12	1:B:142:LEU:HD21	1.58	0.83
1:C:234:LEU:HD22	1:C:520:ASP:HB3	1.61	0.81
1:A:274:SER:HB3	1:A:278:THR:HG21	1.59	0.81
1:B:166:THR:HG21	1:B:214:ALA:HB1	1.65	0.78
1:C:143:LEU:HD12	1:C:212:THR:HG22	1.64	0.78
1:C:278:THR:HG22	1:C:425:GLU:HG3	1.64	0.78
1:B:208:ILE:O	1:B:212:THR:HG23	1.86	0.76
1:D:407:MET:HE3	1:D:411:LEU:CD2	2.17	0.75
1:D:141:ASP:OD1	1:D:197:LYS:CE	2.35	0.74
1:A:263:VAL:HG12	1:A:500:CYS:HB3	1.69	0.74
1:B:176:LYS:HZ1	1:B:183:ARG:HE	1.34	0.73
1:D:188:THR:HG22	1:D:189:THR:HG23	1.69	0.73
1:A:210:LEU:HD12	1:A:213:GLN:NE2	2.03	0.73
1:D:407:MET:CE	1:D:411:LEU:CD2	2.67	0.71
1:C:361:PHE:HE1	1:C:447:VAL:HG12	1.57	0.70
1:B:541:ASP:CG	1:B:543:ARG:NH1	2.48	0.70
1:A:234:LEU:HD22	1:A:520:ASP:HB3	1.74	0.69
1:A:178:CYS:O	1:A:182:LEU:HD12	1.92	0.69
1:D:234:LEU:HD22	1:D:520:ASP:HB3	1.75	0.69
1:D:343:SER:OG	1:D:401:PHE:CD1	2.43	0.68
1:C:295:ILE:HG12	1:C:361:PHE:CD2	2.28	0.68
1:C:524:LEU:HD23	1:C:525:CYS:SG	2.34	0.68
1:B:197:LYS:O	1:B:201:LYS:HB2	1.94	0.67
1:D:361:PHE:HE1	1:D:447:VAL:HG12	1.59	0.67
1:D:488:ILE:HD12	1:D:514:GLY:HA3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:LYS:NZ	1:B:183:ARG:HE	1.91	0.66
1:B:263:VAL:HG12	1:B:500:CYS:HB3	1.76	0.66
1:A:202:LYS:O	1:A:202:LYS:HG3	1.95	0.66
1:A:169:ARG:NH1	1:A:272:ARG:HH11	1.93	0.65
1:B:143:LEU:HD12	1:B:208:ILE:HD11	1.77	0.65
1:C:208:ILE:O	1:C:212:THR:HG23	1.97	0.65
1:B:234:LEU:HD22	1:B:520:ASP:HB3	1.78	0.64
1:D:249:TYR:O	1:D:250:ILE:HD13	1.97	0.64
1:A:145:TYR:CZ	1:A:197:LYS:NZ	2.65	0.64
1:B:170:THR:HB	1:B:179:MET:HE2	1.80	0.64
1:A:139:LEU:HA	1:A:142:LEU:CD2	2.28	0.64
1:A:169:ARG:NH1	1:A:272:ARG:NH1	2.46	0.63
1:B:202:LYS:NZ	1:C:374:SER:HA	2.13	0.63
1:A:210:LEU:HA	1:A:213:GLN:NE2	2.12	0.63
1:A:209:VAL:O	1:A:213:GLN:HG2	1.98	0.63
1:B:216:ARG:O	1:B:216:ARG:HG3	1.97	0.63
1:D:407:MET:HE2	1:D:407:MET:O	1.99	0.62
1:B:216:ARG:HG2	1:B:218:LYS:CE	2.26	0.62
1:C:186:LEU:HD23	1:C:193:VAL:HG21	1.82	0.62
1:B:148:ALA:O	1:B:149:GLU:HB3	2.00	0.62
1:B:139:LEU:CD1	1:B:142:LEU:HD21	2.30	0.61
1:D:361:PHE:CE1	1:D:447:VAL:HG12	2.36	0.60
1:A:210:LEU:HA	1:A:213:GLN:HE21	1.67	0.60
1:B:153:LYS:HB2	1:B:194:MET:HE3	1.84	0.60
1:A:272:ARG:NH1	1:A:369:GLU:OE1	2.33	0.60
1:A:285:GLN:O	1:A:288:VAL:HG22	2.02	0.60
1:D:224:PHE:O	1:D:228:THR:HG23	2.02	0.60
1:B:202:LYS:HA	1:B:205:GLN:HG2	1.84	0.59
1:D:477:GLY:O	1:D:529:ASN:HB2	2.01	0.59
1:B:502:SER:OG	1:B:513:LYS:HE2	2.03	0.59
1:C:498:MET:HE1	1:C:517:PHE:CE2	2.38	0.59
1:D:216:ARG:HE	1:D:216:ARG:HA	1.68	0.59
1:A:155:PRO:HG3	1:A:194:MET:HE3	1.85	0.58
1:B:144:PHE:CE1	1:B:197:LYS:HG2	2.39	0.58
1:D:289:LYS:HD3	1:D:338:ALA:HB2	1.86	0.57
1:B:317:ARG:HA	1:B:319:ASN:CG	2.30	0.56
1:D:496:MET:HE3	1:D:498:MET:SD	2.45	0.56
1:B:250:ILE:HD11	1:B:253:LEU:HB2	1.86	0.56
1:C:145:TYR:N	3:C:601:HOH:O	2.33	0.56
1:D:317:ARG:HA	1:D:319:ASN:ND2	2.20	0.56
1:C:140:GLU:O	3:C:601:HOH:O	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ILE:CG2	1:D:154:ILE:HD13	2.35	0.56
1:D:139:LEU:HD22	1:D:139:LEU:H	1.70	0.56
1:C:250:ILE:HB	1:C:380:SER:OG	2.06	0.55
1:D:295:ILE:HG12	1:D:361:PHE:CD2	2.41	0.55
1:C:340:VAL:O	1:C:343:SER:HB3	2.07	0.55
1:A:145:TYR:CE1	1:A:197:LYS:NZ	2.73	0.55
1:A:170:THR:HB	1:A:179:MET:HE2	1.89	0.55
1:C:346:LYS:O	1:C:354:LYS:NZ	2.40	0.55
1:D:252:GLN:HE21	1:D:376:ALA:HB1	1.71	0.55
1:C:488:ILE:HD12	1:C:514:GLY:HA3	1.88	0.55
1:B:139:LEU:HD12	1:B:142:LEU:CD2	2.31	0.55
1:C:349:VAL:CG1	1:C:353:GLU:HB2	2.37	0.55
1:C:153:LYS:HB3	1:C:194:MET:HB3	1.89	0.54
1:B:387:ARG:O	1:B:391:ILE:HG13	2.08	0.54
1:C:267:THR:HA	1:C:496:MET:HA	1.88	0.54
1:D:249:TYR:CE1	1:D:250:ILE:HG12	2.43	0.54
1:A:245:LYS:HG3	3:A:601:HOH:O	2.06	0.54
1:C:274:SER:HB3	1:C:278:THR:HG21	1.89	0.54
1:C:188:THR:HG22	1:C:189:THR:HG23	1.90	0.53
1:C:382:ARG:O	1:C:382:ARG:HG2	2.08	0.53
1:A:224:PHE:O	1:A:228:THR:HG23	2.09	0.53
1:D:250:ILE:HB	1:D:253:LEU:HD23	1.90	0.53
1:C:191:ASP:O	1:C:191:ASP:OD2	2.26	0.53
1:B:248:ASP:OD1	1:B:249:TYR:N	2.42	0.53
1:D:141:ASP:OD2	1:D:197:LYS:HE3	2.08	0.53
1:A:169:ARG:HH11	1:A:272:ARG:HH11	1.57	0.53
1:C:291:LEU:HD23	1:C:362:LEU:HD22	1.91	0.52
1:A:402:PRO:O	1:A:405:THR:OG1	2.21	0.52
1:B:178:CYS:O	1:B:182:LEU:HD12	2.09	0.52
1:A:267:THR:HA	1:A:496:MET:HA	1.92	0.52
1:C:140:GLU:OE2	1:C:201:LYS:HG2	2.09	0.52
1:A:169:ARG:CD	1:A:272:ARG:HE	2.23	0.52
1:B:140:GLU:HB2	1:B:201:LYS:HG2	1.91	0.52
1:A:210:LEU:CD1	1:A:213:GLN:HE21	2.16	0.52
1:B:498:MET:HE1	1:B:517:PHE:CE1	2.44	0.52
1:C:182:LEU:HD23	1:C:203:CYS:SG	2.50	0.52
1:C:224:PHE:O	1:C:228:THR:HG23	2.09	0.52
1:C:477:GLY:O	1:C:529:ASN:HB2	2.09	0.52
1:A:153:LYS:HB3	1:A:194:MET:HB3	1.92	0.51
1:A:522:VAL:O	1:A:539:LYS:HE2	2.10	0.51
1:B:317:ARG:HA	1:B:319:ASN:ND2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:SER:HA	1:D:383:GLU:HG2	1.93	0.51
1:C:490:LEU:HB3	1:C:498:MET:HB2	1.93	0.50
1:B:317:ARG:NH1	1:B:317:ARG:HG2	2.26	0.50
1:B:349:VAL:O	1:B:354:LYS:HE3	2.12	0.50
1:C:193:VAL:HG23	1:C:193:VAL:O	2.11	0.50
1:D:446:ARG:NH1	3:D:701:HOH:O	2.38	0.50
1:B:289:LYS:HD3	1:B:338:ALA:HB2	1.92	0.50
1:B:267:THR:HA	1:B:496:MET:HA	1.94	0.50
1:C:144:PHE:HB2	1:C:200:PHE:CD2	2.46	0.50
1:C:185:THR:HA	1:C:188:THR:HB	1.93	0.50
1:C:457:LEU:HD21	1:C:491:VAL:HG11	1.94	0.50
1:A:182:LEU:O	1:A:186:LEU:HD12	2.12	0.49
1:C:143:LEU:HD22	1:C:200:PHE:HZ	1.77	0.49
1:A:477:GLY:O	1:A:529:ASN:HB2	2.11	0.49
1:C:249:TYR:CD1	1:C:250:ILE:HG23	2.47	0.49
1:C:289:LYS:HA	1:C:292:LYS:HE2	1.95	0.49
1:C:506:ASP:HB3	1:C:512:VAL:HG12	1.94	0.49
1:D:153:LYS:HB3	1:D:194:MET:HB3	1.93	0.49
1:A:139:LEU:HA	1:A:142:LEU:HD22	1.94	0.49
1:C:201:LYS:O	1:C:205:GLN:HB3	2.12	0.49
1:D:147:ILE:O	1:D:158:LYS:HE2	2.12	0.49
1:D:329:PRO:HG2	1:D:340:VAL:HG21	1.94	0.49
1:D:147:ILE:O	1:D:147:ILE:HG22	2.13	0.49
1:A:178:CYS:O	1:A:182:LEU:CD1	2.61	0.49
1:A:162:ALA:HB1	1:A:215:PHE:HE1	1.78	0.48
1:B:142:LEU:HG	1:B:143:LEU:N	2.27	0.48
1:D:462:SER:O	1:D:469:SER:HB3	2.13	0.48
1:D:185:THR:HA	1:D:188:THR:HB	1.95	0.48
1:B:253:LEU:HD11	1:B:485:ALA:HA	1.95	0.48
1:B:332:PRO:HD2	1:B:459:LEU:HD13	1.96	0.48
1:A:148:ALA:HA	1:A:154:ILE:HG12	1.95	0.48
1:A:490:LEU:HB3	1:A:498:MET:HB2	1.94	0.48
1:C:278:THR:HG22	1:C:425:GLU:CG	2.41	0.48
1:D:349:VAL:O	1:D:354:LYS:HE3	2.12	0.48
1:B:299:ASP:OD2	1:B:357:TYR:OH	2.31	0.48
1:B:477:GLY:O	1:B:529:ASN:HB2	2.14	0.48
1:C:253:LEU:HD21	1:C:285:GLN:HE21	1.79	0.48
1:C:492:VAL:HG21	1:C:496:MET:HE2	1.96	0.48
1:D:322:PHE:O	1:D:323:LEU:HD23	2.14	0.48
1:D:286:SER:HB3	1:D:289:LYS:HZ2	1.78	0.47
1:B:323:LEU:HD21	1:B:395:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:ARG:HD2	1:D:528:HIS:CD2	2.49	0.47
1:B:461:HIS:HE1	1:D:461:HIS:CD2	2.33	0.47
1:B:143:LEU:O	1:B:147:ILE:HG13	2.14	0.47
1:B:365:MET:HG3	1:B:447:VAL:HG11	1.95	0.47
1:C:286:SER:O	1:C:289:LYS:HG3	2.15	0.47
1:B:140:GLU:CB	1:B:201:LYS:HG2	2.45	0.47
1:B:374:SER:HB2	1:B:421:GLU:OE2	2.13	0.47
1:A:302:THR:OG1	1:A:455:ASN:OD1	2.30	0.47
1:A:427:ALA:HB3	1:A:499:MET:HG2	1.97	0.47
1:B:156:VAL:CG2	1:B:182:LEU:HD22	2.45	0.47
1:D:302:THR:OG1	1:D:455:ASN:OD1	2.28	0.47
1:D:480:ALA:HB2	1:D:490:LEU:HD12	1.95	0.47
1:A:289:LYS:HD3	1:A:338:ALA:HB2	1.97	0.47
1:A:307:ARG:O	1:A:328:LYS:HD3	2.15	0.47
1:B:153:LYS:HB3	1:B:194:MET:HB3	1.97	0.47
1:D:407:MET:SD	1:D:407:MET:C	2.98	0.46
1:A:365:MET:HG3	1:A:447:VAL:HG11	1.96	0.46
1:A:169:ARG:HD2	1:A:272:ARG:HE	1.80	0.46
1:A:210:LEU:CD1	1:A:213:GLN:NE2	2.76	0.46
1:C:346:LYS:HE2	1:C:357:TYR:CD1	2.50	0.46
1:B:364:LYS:NZ	3:B:701:HOH:O	2.46	0.46
1:C:186:LEU:CD2	1:C:193:VAL:HG21	2.45	0.46
1:D:286:SER:O	1:D:289:LYS:HG3	2.16	0.46
1:D:349:VAL:CG1	1:D:353:GLU:HB2	2.44	0.46
1:C:264:SER:HB2	1:C:428:SER:HB3	1.97	0.46
1:C:274:SER:CB	1:C:278:THR:HG21	2.46	0.46
1:A:140:GLU:CB	1:A:201:LYS:HG2	2.46	0.46
1:C:143:LEU:HD23	1:C:143:LEU:O	2.15	0.46
1:C:266:CYS:O	1:C:432:ALA:HB2	2.16	0.46
1:B:317:ARG:HG2	1:B:317:ARG:O	2.16	0.46
1:B:479:PRO:HD2	1:B:491:VAL:O	2.16	0.46
1:D:192:GLY:HA3	1:D:193:VAL:HA	1.39	0.46
1:B:365:MET:HE2	1:B:448:LEU:HD11	1.98	0.45
1:D:174:ARG:NH1	1:D:269:ASP:O	2.43	0.45
1:D:261:TRP:HA	1:D:501:TRP:O	2.16	0.45
1:D:286:SER:HB3	1:D:289:LYS:NZ	2.31	0.45
1:A:202:LYS:O	1:A:202:LYS:CG	2.57	0.45
1:B:228:THR:HB	1:B:273:HIS:CE1	2.51	0.45
1:C:354:LYS:HB3	1:C:413:PHE:CZ	2.50	0.45
1:A:192:GLY:HA3	1:A:193:VAL:HA	1.60	0.45
1:C:143:LEU:HD22	1:C:200:PHE:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:CYS:HA	1:D:203:CYS:O	2.16	0.45
1:C:144:PHE:HD1	1:C:200:PHE:CG	2.33	0.45
1:D:332:PRO:HD2	1:D:459:LEU:HD13	1.99	0.45
1:D:422:VAL:HG21	1:D:427:ALA:HB2	1.99	0.45
1:C:186:LEU:O	1:C:186:LEU:CD1	2.58	0.45
1:C:349:VAL:HG11	1:C:353:GLU:HB2	1.98	0.45
1:C:361:PHE:CE1	1:C:447:VAL:HG12	2.45	0.45
1:D:201:LYS:O	1:D:205:GLN:HB2	2.17	0.45
1:B:248:ASP:HA	1:B:254:ALA:HB2	1.99	0.45
1:D:165:SER:HB2	1:D:225:MET:SD	2.56	0.45
1:D:365:MET:HE2	1:D:448:LEU:HD11	1.99	0.45
1:C:252:GLN:NE2	1:C:376:ALA:O	2.50	0.45
1:D:340:VAL:O	1:D:343:SER:HB2	2.17	0.45
1:D:250:ILE:HG22	1:D:252:GLN:H	1.82	0.45
1:A:304:TYR:CD1	1:A:304:TYR:C	2.94	0.44
1:C:153:LYS:HG2	1:C:194:MET:HB3	1.99	0.44
1:C:361:PHE:CD1	1:C:365:MET:HE3	2.52	0.44
1:D:268:VAL:HG13	1:D:436:ASN:CG	2.41	0.44
1:A:498:MET:HE1	1:A:517:PHE:CE2	2.53	0.44
1:B:156:VAL:HG11	1:B:186:LEU:HD11	1.99	0.44
1:C:365:MET:HE2	1:C:448:LEU:HD11	1.98	0.44
1:D:392:GLY:HA3	1:D:407:MET:HE3	1.98	0.44
1:B:148:ALA:O	1:B:151:GLN:HB2	2.17	0.44
1:C:261:TRP:HA	1:C:501:TRP:O	2.18	0.44
1:D:140:GLU:OE1	1:D:140:GLU:N	2.36	0.44
1:A:507:LYS:HG2	1:A:507:LYS:O	2.18	0.44
1:B:528:HIS:CD2	1:D:454:ARG:HD2	2.53	0.44
1:D:147:ILE:HG22	1:D:154:ILE:HD13	2.00	0.44
1:D:228:THR:HB	1:D:273:HIS:CE1	2.52	0.44
1:A:180:ASP:OD1	1:A:183:ARG:NH1	2.51	0.44
1:C:192:GLY:HA3	1:C:193:VAL:HA	1.38	0.44
1:C:268:VAL:HG12	1:C:436:ASN:HB2	1.99	0.44
1:A:268:VAL:HG12	1:A:436:ASN:HB2	1.99	0.43
1:A:316:LEU:HD12	1:A:316:LEU:HA	1.86	0.43
1:B:346:LYS:HA	1:B:346:LYS:HD2	1.88	0.43
1:B:320:LYS:HA	1:B:320:LYS:HD3	1.51	0.43
1:C:281:PRO:HA	1:C:422:VAL:O	2.19	0.43
1:C:313:PRO:HG3	1:C:462:SER:HB2	2.00	0.43
1:C:196:ASP:OD1	1:C:196:ASP:N	2.51	0.43
1:D:164:LYS:HB3	1:D:164:LYS:HE3	1.76	0.43
1:C:138:SER:OG	1:C:141:ASP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:LYS:O	1:B:176:LYS:HG3	2.19	0.43
1:A:140:GLU:HB3	1:A:201:LYS:HG2	2.00	0.43
1:A:362:LEU:HB3	1:A:430:MET:CE	2.49	0.43
1:B:479:PRO:HG3	1:D:530:TYR:CE1	2.54	0.43
1:B:524:LEU:HD23	1:B:525:CYS:SG	2.59	0.43
1:A:529:ASN:ND2	1:A:530:TYR:CE2	2.87	0.43
1:B:407:MET:SD	1:B:411:LEU:HD23	2.58	0.43
1:C:479:PRO:HD2	1:C:491:VAL:O	2.19	0.42
1:A:160:ILE:O	1:A:164:LYS:HG3	2.18	0.42
1:C:364:LYS:HE2	1:C:445:GLU:OE2	2.19	0.42
1:D:195:LEU:HD23	1:D:199:LEU:HD23	2.02	0.42
1:A:349:VAL:O	1:A:354:LYS:HE3	2.19	0.42
1:B:268:VAL:HG12	1:B:436:ASN:HB2	2.01	0.42
1:C:196:ASP:HB2	1:C:198:ASP:OD1	2.19	0.42
1:B:250:ILE:HD12	1:B:252:GLN:HB2	2.01	0.42
1:A:293:TYR:OH	1:A:306:HIS:NE2	2.34	0.42
1:A:449:SER:O	1:A:453:VAL:HG23	2.19	0.42
1:A:502:SER:OG	1:A:513:LYS:NZ	2.45	0.42
1:B:192:GLY:HA3	1:B:193:VAL:HA	1.77	0.42
1:D:379:GLN:O	1:D:383:GLU:HB3	2.20	0.42
1:A:188:THR:HG22	1:A:189:THR:HG23	2.02	0.42
1:A:522:VAL:CG1	1:A:528:HIS:HB2	2.50	0.42
1:B:252:GLN:N	1:B:252:GLN:CD	2.78	0.42
1:D:192:GLY:N	1:D:193:VAL:HG22	2.35	0.42
1:D:540:LEU:HD12	1:D:540:LEU:HA	1.89	0.42
1:B:181:MET:HE2	1:B:181:MET:HB2	1.96	0.42
1:D:183:ARG:O	1:D:187:GLN:HG3	2.20	0.42
1:D:228:THR:HB	1:D:273:HIS:ND1	2.35	0.42
1:B:220:VAL:N	1:B:269:ASP:OD2	2.48	0.42
1:B:525:CYS:HA	1:B:540:LEU:O	2.19	0.42
1:D:145:TYR:HB3	1:D:146:THR:H	1.59	0.42
1:D:176:LYS:HD2	1:D:176:LYS:HA	1.95	0.42
1:B:289:LYS:HA	1:B:292:LYS:HE2	2.02	0.41
1:B:144:PHE:O	1:B:148:ALA:HB2	2.20	0.41
1:A:157:HIS:O	1:A:161:THR:HG23	2.21	0.41
1:B:187:GLN:O	1:B:188:THR:C	2.63	0.41
1:A:143:LEU:HD12	1:A:212:THR:HG22	2.01	0.41
1:C:316:LEU:HA	1:C:316:LEU:HD23	1.78	0.41
1:B:274:SER:HB3	1:B:278:THR:HG21	2.01	0.41
1:C:323:LEU:HD12	1:C:394:TYR:HE2	1.86	0.41
1:B:272:ARG:HH12	1:B:369:GLU:CD	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LYS:O	1:A:201:LYS:HB2	2.21	0.41
1:C:235:TYR:HD1	1:C:236:GLU:HG2	1.86	0.41
1:C:257:SER:HA	1:C:258:PRO:HD3	1.95	0.41
1:A:165:SER:HB2	1:A:225:MET:SD	2.60	0.41
1:A:410:ILE:HD13	1:A:410:ILE:HA	1.93	0.41
1:A:525:CYS:C	1:A:527:PHE:H	2.28	0.41
1:B:365:MET:HE2	1:B:448:LEU:HD21	2.03	0.41
1:C:144:PHE:O	1:C:148:ALA:HB2	2.21	0.41
1:B:160:ILE:HD12	1:B:161:THR:N	2.36	0.40
1:C:498:MET:HE1	1:C:517:PHE:HE2	1.84	0.40
1:C:358:VAL:O	1:C:362:LEU:HG	2.21	0.40
1:D:249:TYR:CD1	1:D:250:ILE:HG12	2.56	0.40
1:D:388:ASN:HB3	1:D:411:LEU:HD11	2.02	0.40
1:A:364:LYS:NZ	3:A:603:HOH:O	2.54	0.40
1:C:140:GLU:C	1:C:142:LEU:N	2.77	0.40
1:D:158:LYS:HD3	1:D:158:LYS:C	2.45	0.40
1:B:142:LEU:CD1	1:B:216:ARG:NH2	2.84	0.40
1:B:261:TRP:HA	1:B:501:TRP:O	2.21	0.40
1:B:325:GLU:OE1	1:D:317:ARG:HB2	2.22	0.40
1:C:435:ALA:HB2	1:C:491:VAL:HG13	2.02	0.40
1:C:507:LYS:HD2	1:C:507:LYS:HA	1.88	0.40
1:D:250:ILE:HD13	1:D:250:ILE:HA	1.86	0.40
1:D:417:LEU:HD23	1:D:417:LEU:HA	1.92	0.40
1:A:224:PHE:HB2	1:A:271:GLN:NE2	2.36	0.40
1:B:232:ASP:O	1:B:236:GLU:HG2	2.21	0.40
1:C:449:SER:O	1:C:453:VAL:HG23	2.22	0.40
1:D:498:MET:HB3	1:D:498:MET:HE2	1.73	0.40

All (1) 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:A:307:ARG:NH2	1:B:259:ASP:OD1[1_655]	2.11	0.09

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	399/527 (76%)	374 (94%)	24 (6%)	1 (0%)	36	60
1	B	407/527 (77%)	388 (95%)	17 (4%)	2 (0%)	24	48
1	C	408/527 (77%)	390 (96%)	17 (4%)	1 (0%)	43	68
1	D	407/527 (77%)	386 (95%)	20 (5%)	1 (0%)	43	68
All	All	1621/2108 (77%)	1538 (95%)	78 (5%)	5 (0%)	36	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	SER
1	B	188	THR
1	C	141	ASP
1	D	145	TYR
1	B	151	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	349/452 (77%)	349 (100%)	0	100	100
1	B	354/452 (78%)	354 (100%)	0	100	100
1	C	354/452 (78%)	354 (100%)	0	100	100
1	D	354/452 (78%)	354 (100%)	0	100	100
All	All	1411/1808 (78%)	1411 (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	205	GLN
1	A	213	GLN
1	A	335	ASN
1	A	347	GLN
1	A	388	ASN
1	A	416	GLN
1	A	535	HIS
1	B	187	GLN
1	B	271	GLN
1	B	347	GLN
1	B	461	HIS
1	B	529	ASN
1	C	271	GLN
1	C	285	GLN
1	C	455	ASN
1	C	471	GLN
1	C	529	ASN
1	C	535	HIS
1	D	510	ASN
1	D	535	HIS

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	QAJ	D	601	-	41,41,41	0.83	0	51,55,55	2.39	16 (31%)
2	QAJ	B	601	-	41,41,41	0.87	0	51,55,55	2.88	19 (37%)

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	QAJ	D	601	-	-	13/24/34/34	1/5/5/5
2	QAJ	B	601	-	-	11/24/34/34	0/5/5/5

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	QAJ	C5-N2-C6	-10.97	105.22	124.48
2	D	601	QAJ	N9-C16-N8	8.12	128.07	120.81
2	B	601	QAJ	N5-C7-N4	7.42	127.44	120.81
2	D	601	QAJ	N1-C15-N7	5.53	127.60	116.91
2	D	601	QAJ	N5-C7-N4	5.43	125.67	120.81
2	D	601	QAJ	C2-N1-C15	-5.06	109.28	122.09
2	B	601	QAJ	C2-N1-C15	-4.95	109.54	122.09
2	B	601	QAJ	C3-C4-C5	-4.94	102.87	110.67
2	B	601	QAJ	C2-C1-C5	-4.78	103.13	110.67
2	B	601	QAJ	N1-C15-N7	4.74	126.08	116.91
2	B	601	QAJ	N9-C16-N8	4.44	124.78	120.81
2	D	601	QAJ	S2-C16-N9	-4.38	117.86	123.72
2	D	601	QAJ	C5-N2-C6	-3.83	117.75	124.48
2	B	601	QAJ	C1-C5-C4	-3.70	104.42	110.80
2	B	601	QAJ	C4-C5-N2	3.67	117.91	110.57
2	D	601	QAJ	C9-C8-N5	-3.45	110.19	114.40
2	B	601	QAJ	S1-C7-N5	-3.39	119.18	123.72
2	B	601	QAJ	C15-N7-N8	3.35	113.70	107.08
2	D	601	QAJ	C15-N7-N8	2.98	112.96	107.08
2	D	601	QAJ	O2-C17-C18	-2.90	115.70	121.99
2	D	601	QAJ	C8-N5-C7	-2.86	118.79	123.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	QAJ	S1-C7-N5	-2.80	119.97	123.72
2	B	601	QAJ	C18-C17-N9	-2.68	111.13	114.40
2	B	601	QAJ	C9-C8-N5	-2.66	111.16	114.40
2	B	601	QAJ	C21-C20-C19	-2.63	116.92	120.61
2	D	601	QAJ	C21-C20-C19	-2.44	117.17	120.61
2	B	601	QAJ	O2-C17-N9	2.43	127.05	122.44
2	B	601	QAJ	S1-C6-N3	-2.40	111.85	114.52
2	D	601	QAJ	C10-C9-C8	-2.22	105.69	112.33
2	B	601	QAJ	C3-N1-C15	-2.16	116.62	122.09
2	B	601	QAJ	S2-C16-N9	-2.16	120.83	123.72
2	D	601	QAJ	O1-C8-C9	-2.06	117.52	121.99
2	B	601	QAJ	C17-N9-C16	-2.05	120.17	123.69
2	D	601	QAJ	C19-C18-C17	-2.05	106.20	112.33
2	D	601	QAJ	C20-C19-C23	2.03	120.09	117.10

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	QAJ	N7-C15-N1-C2
2	B	601	QAJ	S2-C15-N1-C2
2	B	601	QAJ	N7-C15-N1-C3
2	B	601	QAJ	N3-C6-N2-C5
2	B	601	QAJ	S1-C6-N2-C5
2	B	601	QAJ	N4-C7-N5-C8
2	B	601	QAJ	S1-C7-N5-C8
2	B	601	QAJ	O1-C8-N5-C7
2	D	601	QAJ	N7-C15-N1-C2
2	D	601	QAJ	S2-C15-N1-C2
2	D	601	QAJ	C1-C5-N2-C6
2	D	601	QAJ	N3-C6-N2-C5
2	D	601	QAJ	S1-C6-N2-C5
2	D	601	QAJ	O1-C8-N5-C7
2	D	601	QAJ	O2-C17-N9-C16
2	D	601	QAJ	N8-C16-N9-C17
2	D	601	QAJ	S2-C16-N9-C17
2	B	601	QAJ	S2-C15-N1-C3
2	D	601	QAJ	C9-C8-N5-C7
2	D	601	QAJ	C18-C17-N9-C16
2	D	601	QAJ	S1-C7-N5-C8
2	D	601	QAJ	N4-C7-N5-C8
2	B	601	QAJ	C4-C5-N2-C6

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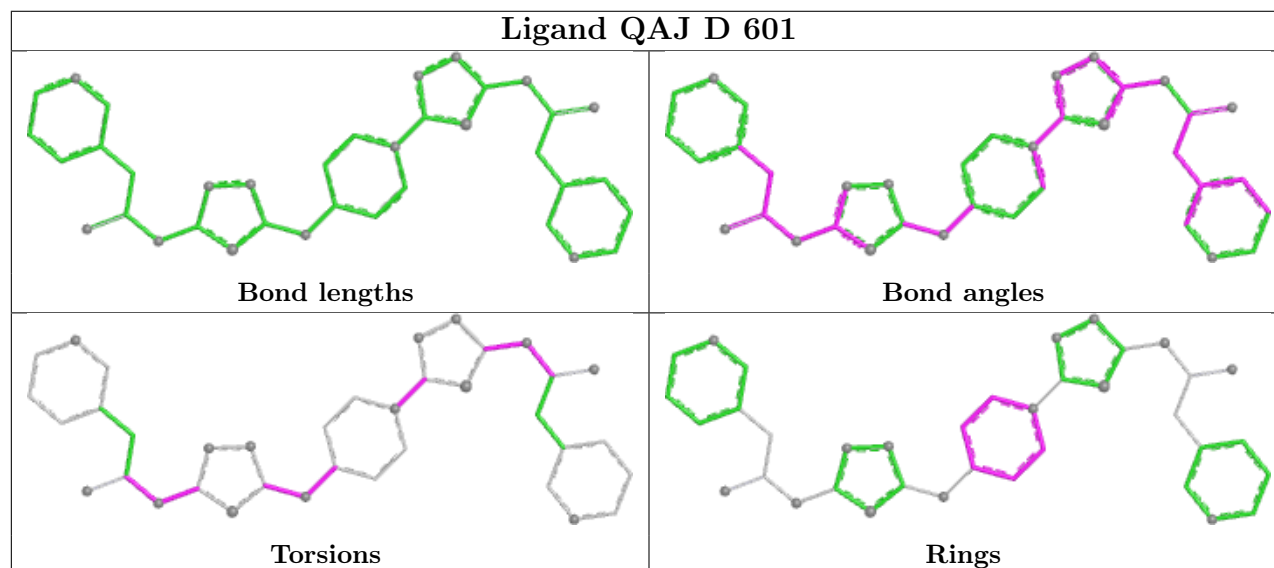
Mol	Chain	Res	Type	Atoms
2	B	601	QAJ	O2-C17-N9-C16

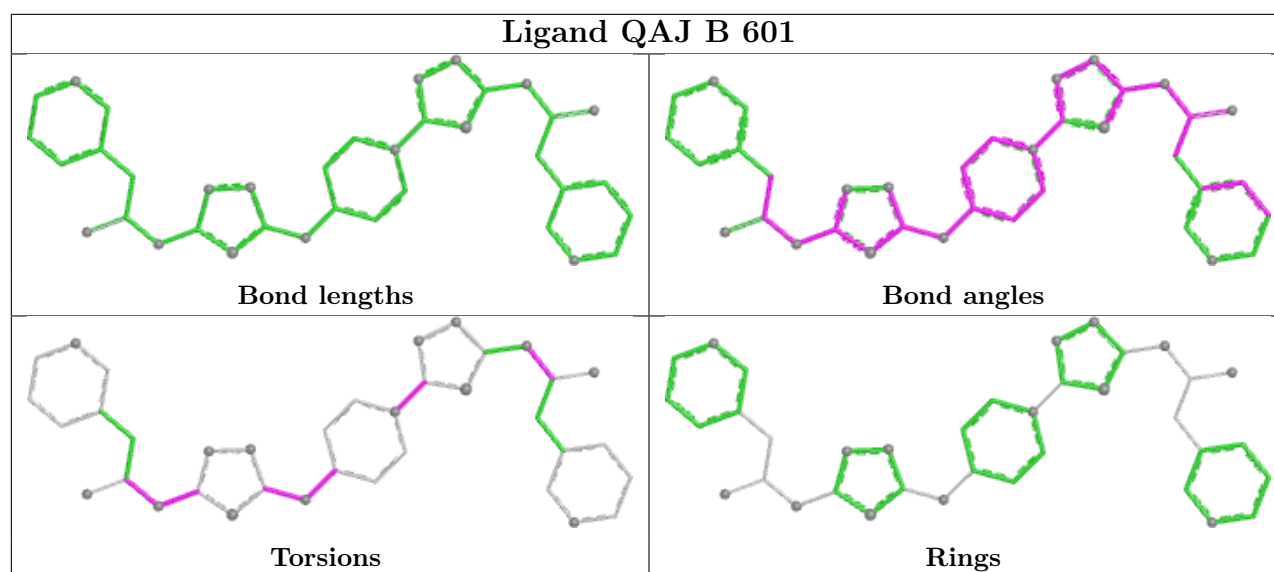
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	QAJ	C1-C2-C3-C4-C5-N1

No monomer is involved in short contacts.

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	403/527 (76%)	0.61	29 (7%) 21 18	38, 56, 113, 164	0
1	B	409/527 (77%)	0.58	31 (7%) 20 17	39, 56, 119, 186	0
1	C	410/527 (77%)	0.71	42 (10%) 12 10	42, 57, 126, 195	0
1	D	409/527 (77%)	0.54	26 (6%) 25 22	38, 55, 110, 166	0
All	All	1631/2108 (77%)	0.61	128 (7%) 19 16	38, 56, 116, 195	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	145	TYR	9.5
1	C	253	LEU	6.2
1	D	318	PHE	6.0
1	C	189	THR	5.4
1	B	318	PHE	4.8
1	C	147	ILE	4.7
1	C	139	LEU	4.6
1	B	141	ASP	4.5
1	B	253	LEU	4.2
1	C	318	PHE	4.1
1	D	139	LEU	4.1
1	C	146	THR	4.1
1	B	189	THR	4.0
1	C	197	LYS	4.0
1	D	145	TYR	4.0
1	B	142	LEU	3.9
1	C	150	GLY	3.9
1	B	202	LYS	3.9
1	B	153	LYS	3.9
1	D	144	PHE	3.9
1	C	137	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	176	LYS	3.8
1	B	188	THR	3.7
1	D	317	ARG	3.7
1	A	148	ALA	3.7
1	B	252	GLN	3.6
1	D	150	GLY	3.6
1	A	145	TYR	3.6
1	C	144	PHE	3.6
1	A	397	GLU	3.6
1	C	325	GLU	3.6
1	D	148	ALA	3.6
1	A	317	ARG	3.5
1	C	249	TYR	3.5
1	B	138	SER	3.5
1	A	279	LYS	3.5
1	B	251	PRO	3.4
1	C	191	ASP	3.4
1	A	318	PHE	3.4
1	D	316	LEU	3.3
1	A	147	ILE	3.2
1	A	189	THR	3.2
1	A	182	LEU	3.2
1	D	193	VAL	3.2
1	D	383	GLU	3.1
1	D	253	LEU	3.1
1	C	256	PHE	3.1
1	B	145	TYR	3.1
1	A	188	THR	3.1
1	C	185	THR	3.1
1	A	137	PRO	3.1
1	D	189	THR	3.1
1	D	137	PRO	3.0
1	D	194	MET	3.0
1	C	546	GLY	3.0
1	B	320	LYS	2.9
1	C	138	SER	2.9
1	C	188	THR	2.9
1	C	151	GLN	2.8
1	A	256	PHE	2.8
1	B	225	MET	2.8
1	C	511	SER	2.8
1	B	146	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	148	ALA	2.8
1	B	137	PRO	2.7
1	B	245	LYS	2.7
1	C	194	MET	2.7
1	D	138	SER	2.7
1	A	245	LYS	2.7
1	C	153	LYS	2.7
1	B	317	ARG	2.6
1	C	209	VAL	2.6
1	A	258	PRO	2.6
1	C	141	ASP	2.6
1	A	198	ASP	2.6
1	D	188	THR	2.6
1	A	225	MET	2.6
1	C	317	ARG	2.5
1	D	225	MET	2.5
1	B	185	THR	2.5
1	C	254	ALA	2.5
1	A	154	ILE	2.5
1	A	205	GLN	2.5
1	D	200	PHE	2.5
1	B	208	ILE	2.4
1	C	383	GLU	2.4
1	A	249	TYR	2.4
1	A	186	LEU	2.4
1	C	169	ARG	2.4
1	B	143	LEU	2.3
1	B	466	TYR	2.3
1	D	185	THR	2.3
1	C	198	ASP	2.3
1	D	254	ALA	2.3
1	A	257	SER	2.3
1	A	500	CYS	2.3
1	A	319	ASN	2.3
1	B	243	GLY	2.3
1	C	387	ARG	2.2
1	A	466	TYR	2.2
1	A	141	ASP	2.2
1	C	143	LEU	2.2
1	C	190	SER	2.2
1	B	160	ILE	2.2
1	C	238	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	176	LYS	2.2
1	C	247	ALA	2.1
1	C	203	CYS	2.1
1	A	202	LYS	2.1
1	C	360	GLN	2.1
1	D	142	LEU	2.1
1	B	191	ASP	2.1
1	B	250	ILE	2.1
1	C	384	SER	2.1
1	B	513	LYS	2.1
1	C	251	PRO	2.1
1	B	178	CYS	2.1
1	D	384	SER	2.1
1	D	153	LYS	2.1
1	C	466	TYR	2.1
1	C	319	ASN	2.1
1	A	224	PHE	2.1
1	A	169	ARG	2.0
1	D	146	THR	2.0
1	D	466	TYR	2.0
1	D	191	ASP	2.0
1	B	166	THR	2.0
1	B	441	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

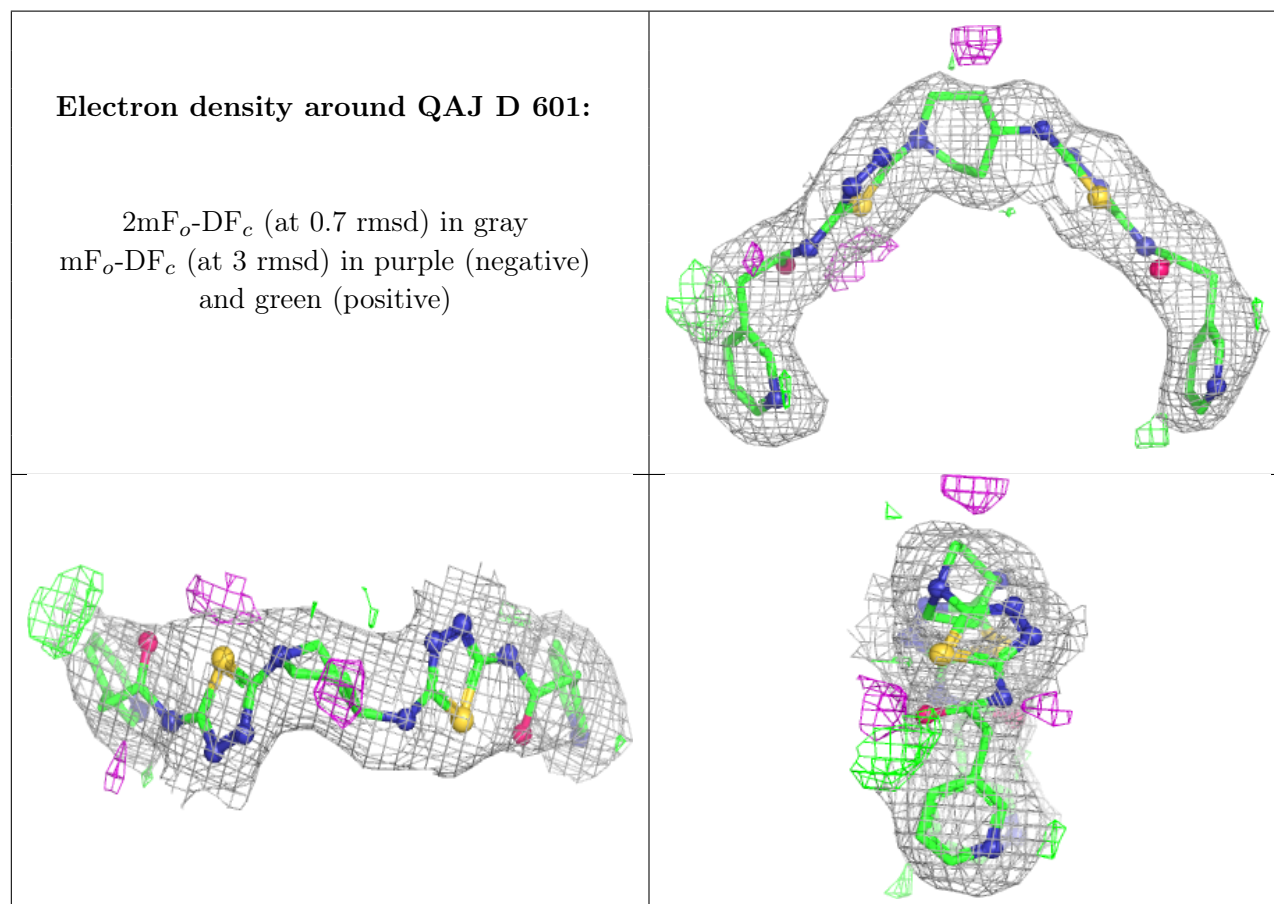
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

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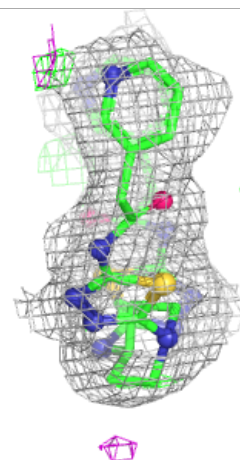
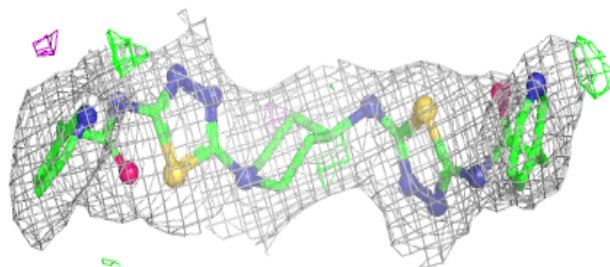
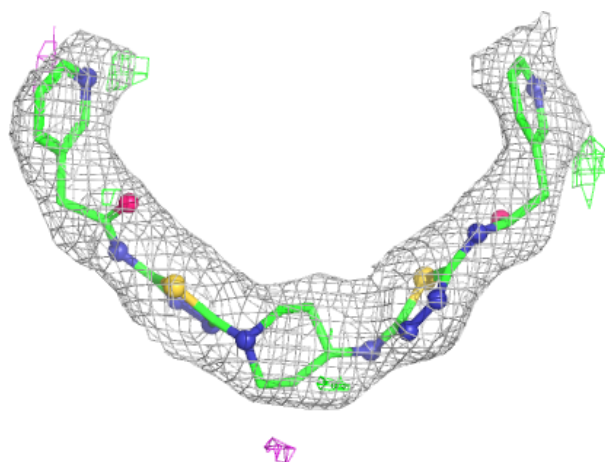
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	QAJ	D	601	37/37	0.90	0.11	39,62,79,83	0
2	QAJ	B	601	37/37	0.92	0.11	52,67,87,89	0

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 QAJ 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.