



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2020 – 11:19 AM EDT

PDB ID : 6UME
Title : Crystal structure of human GAC in complex with inhibitor UPGL00012
Authors : Huang, Q.; Cerione, R.A.
Deposited on : 2019-10-09
Resolution : 2.90 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

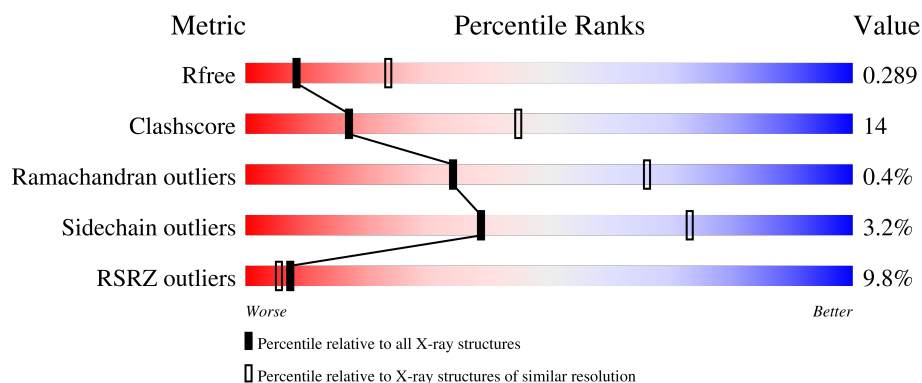
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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>7%</div> <div>58%</div> <div>17%</div> <div>•</div> <div>22%</div> </div>
1	B	527	<div> <div>8%</div> <div>54%</div> <div>22%</div> <div>•</div> <div>22%</div> </div>
1	C	527	<div> <div>9%</div> <div>54%</div> <div>21%</div> <div>•</div> <div>22%</div> </div>
1	D	527	<div> <div>7%</div> <div>54%</div> <div>23%</div> <div>•</div> <div>22%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12846 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.

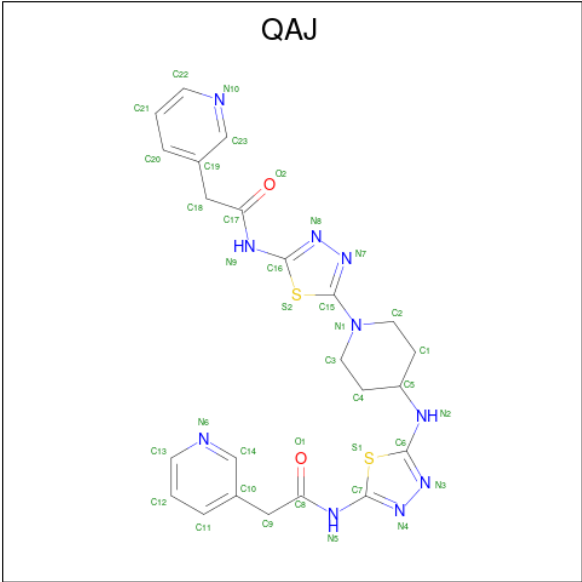
- Molecule 1 is a protein called Glutaminase kidney isoform, mitochondrial.

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 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 (three-letter code: QAJ) (formula: C₂₃H₂₄N₁₀O₂S₂) (labeled as "Ligand of Interest" by author).

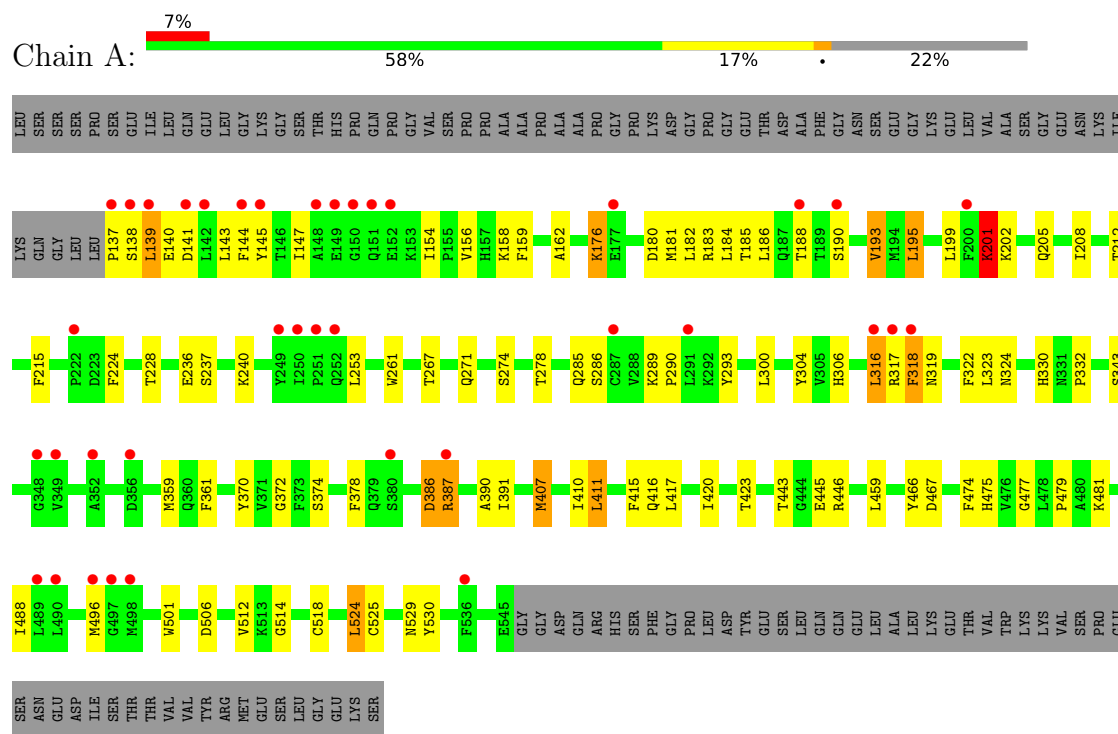


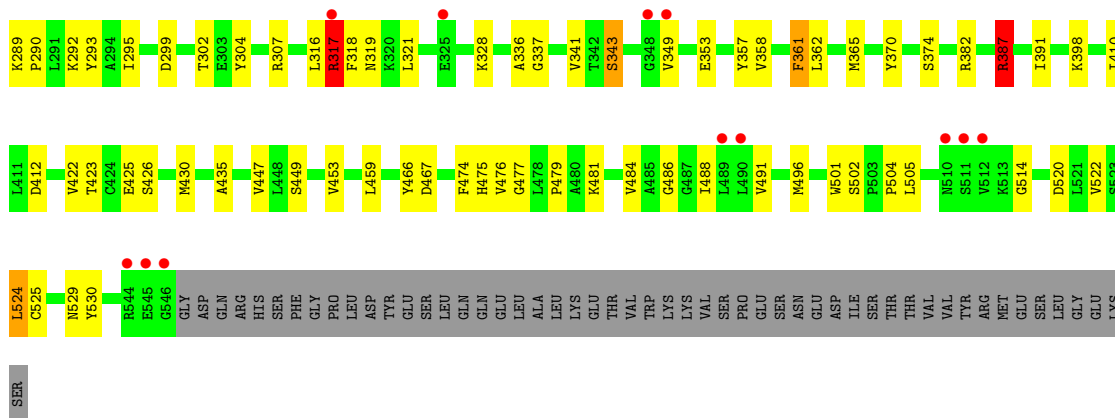
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			37	23	10	2	2		
2	B	1	Total	C	N	O	S	0	0
			37	23	10	2	2		

3 Residue-property plots

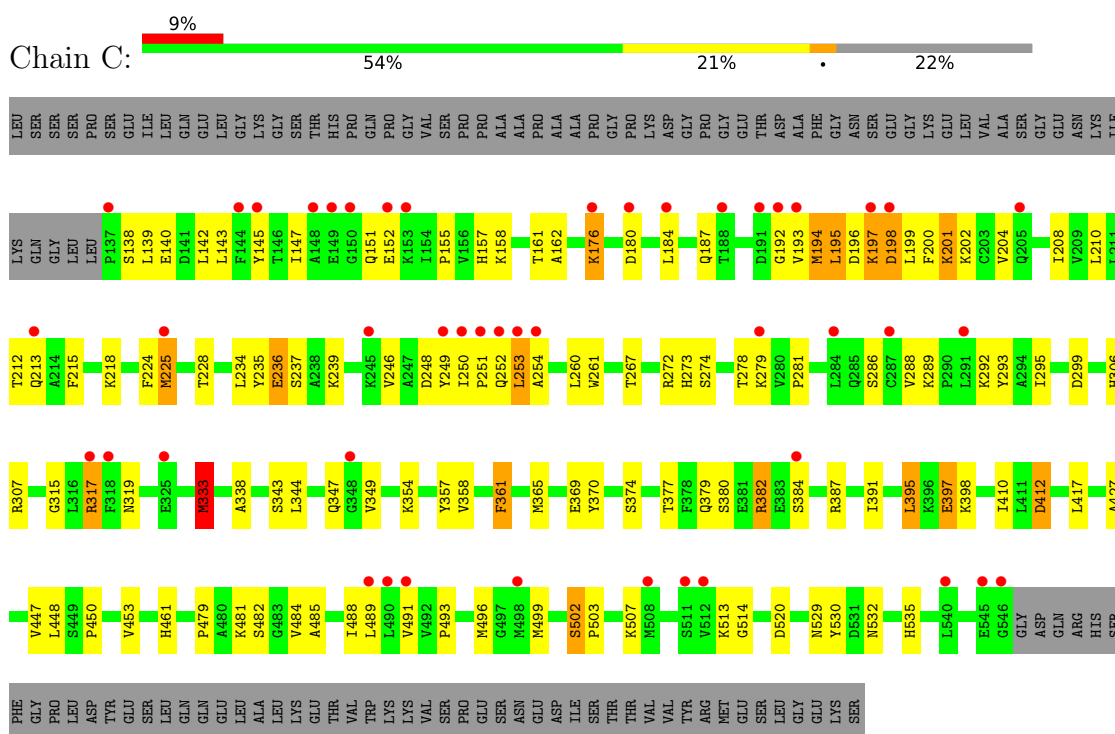
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

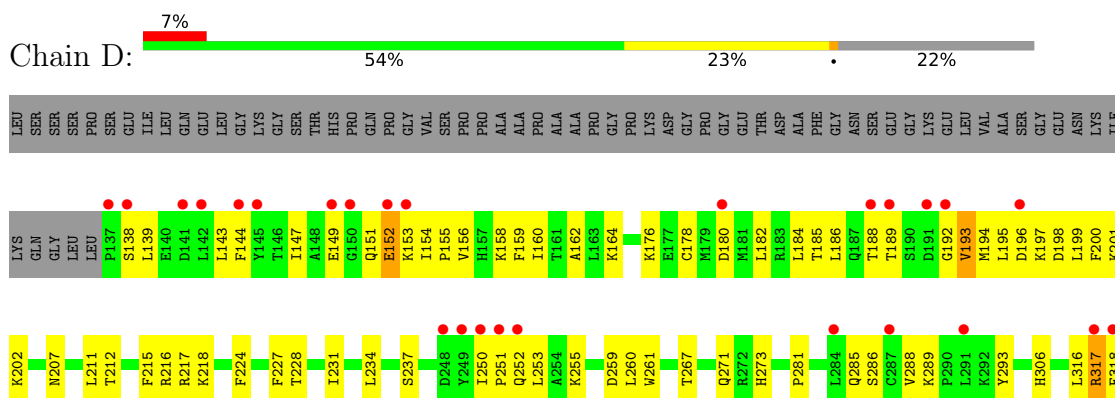


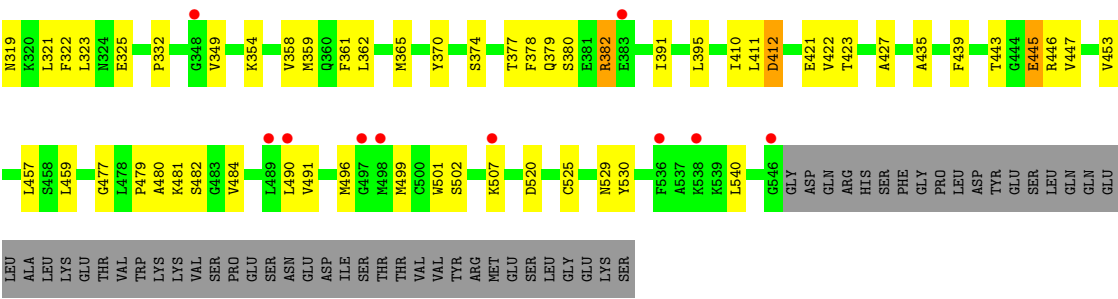


- Molecule 1: Glutaminase kidney isoform, mitochondrial



- Molecule 1: Glutaminase kidney isoform, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.87Å 139.09Å 178.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.46 – 2.90 24.46 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (24.46-2.90) 99.2 (24.46-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.89Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.227 , 0.289 0.227 , 0.289	Depositor DCC
R_{free} test set	1761 reflections (3.16%)	wwPDB-VP
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.985	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12846	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.07 % 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 2.1572e-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 [i](#)

5.1 Standard geometry [i](#)

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	0.56	5/3262 (0.2%)	0.82	12/4403 (0.3%)
1	B	0.50	1/3266 (0.0%)	0.77	5/4408 (0.1%)
1	C	0.60	1/3266 (0.0%)	0.87	22/4408 (0.5%)
1	D	0.51	2/3266 (0.1%)	0.80	6/4408 (0.1%)
All	All	0.54	9/13060 (0.1%)	0.82	45/17627 (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	B	0	1
1	D	0	2
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	397	GLU	CB-CG	11.31	1.73	1.52
1	A	318	PHE	CB-CG	-7.21	1.39	1.51
1	A	387	ARG	CZ-NH2	-6.84	1.24	1.33
1	B	317	ARG	CZ-NH1	6.23	1.41	1.33
1	A	318	PHE	CD1-CE1	-6.22	1.26	1.39
1	D	149	GLU	CB-CG	5.95	1.63	1.52
1	D	317	ARG	CB-CG	5.78	1.68	1.52
1	A	518	CYS	CB-SG	-5.72	1.72	1.81
1	A	318	PHE	CD2-CE2	-5.39	1.28	1.39

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	317	ARG	NE-CZ-NH1	-14.49	113.05	120.30
1	D	149	GLU	CA-CB-CG	9.87	135.11	113.40
1	A	316	LEU	CB-CG-CD2	-9.36	95.08	111.00
1	B	195	LEU	CA-CB-CG	9.29	136.68	115.30
1	C	253	LEU	CB-CG-CD2	8.52	125.48	111.00
1	A	183	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	C	317	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	A	195	LEU	CA-CB-CG	7.92	133.51	115.30
1	C	198	ASP	CB-CG-OD1	-7.79	111.29	118.30
1	D	382	ARG	CB-CG-CD	7.10	130.06	111.60
1	B	191	ASP	CB-CG-OD1	7.06	124.66	118.30
1	A	316	LEU	CA-CB-CG	-6.99	99.21	115.30
1	A	386	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	C	225	MET	CA-CB-CG	6.82	124.89	113.30
1	C	210	LEU	CA-CB-CG	6.77	130.87	115.30
1	A	139	LEU	CB-CG-CD1	6.68	122.36	111.00
1	B	387	ARG	CG-CD-NE	6.66	125.78	111.80
1	D	317	ARG	NE-CZ-NH2	6.65	123.63	120.30
1	C	152	GLU	CA-CB-CG	-6.51	99.09	113.40
1	C	236	GLU	CA-CB-CG	-6.48	99.15	113.40
1	A	201	LYS	CB-CG-CD	-6.44	94.86	111.60
1	A	411	LEU	CA-CB-CG	-6.27	100.88	115.30
1	C	279	LYS	CA-CB-CG	6.25	127.16	113.40
1	A	318	PHE	CB-CG-CD1	-6.23	116.44	120.80
1	C	317	ARG	CG-CD-NE	-6.14	98.89	111.80
1	A	386	ASP	CB-CG-OD1	6.05	123.75	118.30
1	A	201	LYS	CD-CE-NZ	5.86	125.17	111.70
1	D	196	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	C	333	MET	CG-SD-CE	5.81	109.50	100.20
1	C	198	ASP	CB-CG-OD2	5.80	123.52	118.30
1	C	317	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	197	LYS	C-N-CA	5.70	135.94	121.70
1	C	225	MET	CG-SD-CE	-5.68	91.10	100.20
1	C	195	LEU	CA-CB-CG	-5.58	102.46	115.30
1	B	387	ARG	NE-CZ-NH1	-5.57	117.51	120.30
1	D	507	LYS	CA-CB-CG	-5.56	101.17	113.40
1	D	139	LEU	CA-CB-CG	-5.50	102.64	115.30
1	C	489	LEU	CB-CG-CD1	-5.40	101.81	111.00
1	C	387	ARG	CA-CB-CG	5.34	125.15	113.40
1	A	183	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	176	LYS	CB-CA-C	-5.19	100.02	110.40
1	C	198	ASP	N-CA-CB	-5.17	101.28	110.60
1	C	176	LYS	CA-CB-CG	-5.08	102.23	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	195	LEU	CB-CG-CD1	5.07	119.62	111.00
1	C	395	LEU	CB-CG-CD1	-5.02	102.46	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	387	ARG	Sidechain
1	D	316	LEU	Peptide
1	D	445	GLU	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3190	0	3167	77	1
1	B	3194	0	3166	93	7
1	C	3194	0	3170	100	3
1	D	3194	0	3170	107	2
2	A	37	0	0	1	0
2	B	37	0	0	2	7
All	All	12846	0	12673	356	10

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 14.

All (356) 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:407:MET:O	1:A:411:LEU:HD12	1.42	1.15
1:A:316:LEU:HD11	1:A:467:ASP:CG	1.83	0.99
1:C:295:ILE:HG12	1:C:361:PHE:CD2	1.98	0.98
1:D:443:THR:OG1	1:D:445:GLU:HG2	1.72	0.89
1:C:140:GLU:HB3	1:C:201:LYS:HG2	1.59	0.85
1:A:407:MET:HG2	1:A:411:LEU:HD11	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ILE:HD11	1:A:159:PHE:HA	1.61	0.82
1:A:407:MET:O	1:A:411:LEU:CD1	2.28	0.81
1:D:152:GLU:HG2	1:D:153:LYS:HD2	1.63	0.80
1:B:317:ARG:O	1:B:317:ARG:HD3	1.86	0.76
1:D:250:ILE:HD12	1:D:252:GLN:HB2	1.67	0.76
1:D:281:PRO:HB3	1:D:370:TYR:HE2	1.49	0.75
1:B:178:CYS:O	1:B:182:LEU:HD13	1.85	0.75
1:C:289:LYS:HD3	1:C:338:ALA:HB2	1.69	0.75
1:D:207:ASN:O	1:D:211:LEU:HD12	1.86	0.74
1:C:361:PHE:HZ	1:C:448:LEU:HD23	1.53	0.74
1:A:201:LYS:HD2	1:A:201:LYS:C	2.07	0.74
1:A:318:PHE:CZ	1:D:317:ARG:HD3	2.21	0.74
1:C:234:LEU:HD22	1:C:520:ASP:HB3	1.70	0.73
1:A:524:LEU:HD23	1:A:525:CYS:SG	2.29	0.73
1:B:147:ILE:HG22	1:B:158:LYS:NZ	2.04	0.72
1:B:488:ILE:HD12	1:B:514:GLY:HA3	1.70	0.72
1:C:145:TYR:OH	1:C:197:LYS:CE	2.38	0.71
1:C:145:TYR:OH	1:C:197:LYS:NZ	2.22	0.71
1:D:285:GLN:HG3	1:D:484:VAL:HG12	1.72	0.70
1:C:145:TYR:CZ	1:C:197:LYS:NZ	2.59	0.70
1:A:147:ILE:O	1:A:158:LYS:NZ	2.22	0.70
1:C:361:PHE:CZ	1:C:448:LEU:HD23	2.27	0.69
1:D:144:PHE:HE1	1:D:154:ILE:HG13	1.58	0.69
1:B:182:LEU:HD11	1:B:203:CYS:HB3	1.75	0.68
1:B:343:SER:HA	1:B:410:ILE:HD12	1.75	0.68
1:B:236:GLU:HG3	1:B:240:LYS:NZ	2.08	0.68
1:A:201:LYS:O	1:A:205:GLN:HB2	1.94	0.68
1:C:343:SER:HA	1:C:410:ILE:HD12	1.76	0.67
1:B:219:PHE:HB3	1:B:271:GLN:NE2	2.09	0.67
1:C:248:ASP:HA	1:C:254:ALA:HB2	1.77	0.67
1:C:307:ARG:NH2	1:D:259:ASP:OD2	2.22	0.67
1:A:506:ASP:HB3	1:A:512:VAL:HG12	1.77	0.66
1:C:299:ASP:OD2	1:C:357:TYR:OH	2.09	0.66
1:C:361:PHE:HE1	1:C:447:VAL:HG12	1.61	0.66
1:B:208:ILE:O	1:B:212:THR:HG23	1.96	0.65
1:B:236:GLU:HG3	1:B:240:LYS:HZ3	1.60	0.65
1:C:274:SER:HB3	1:C:278:THR:HG21	1.77	0.65
1:B:317:ARG:O	1:B:317:ARG:CD	2.44	0.65
1:C:361:PHE:CD1	1:C:365:MET:HE3	2.32	0.65
1:A:386:ASP:O	1:A:390:ALA:N	2.22	0.65
1:B:274:SER:HB3	1:B:278:THR:HG21	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:PHE:CZ	1:B:231:ILE:HD11	2.33	0.64
1:D:216:ARG:HB3	1:D:218:LYS:HE3	1.80	0.64
1:C:295:ILE:HG12	1:C:361:PHE:CE2	2.32	0.64
1:D:378:PHE:O	1:D:382:ARG:HG2	1.97	0.64
1:A:529:ASN:ND2	1:D:529:ASN:OD1	2.28	0.64
1:C:143:LEU:HD22	1:C:200:PHE:HZ	1.62	0.63
1:D:252:GLN:HB3	1:D:377:THR:HG22	1.79	0.63
1:A:443:THR:OG1	1:A:445:GLU:HG2	1.98	0.63
1:C:481:LYS:NZ	1:C:482:SER:O	2.31	0.63
1:D:144:PHE:CD2	1:D:197:LYS:HG2	2.34	0.63
1:D:153:LYS:HB3	1:D:195:LEU:O	1.99	0.62
1:A:407:MET:HG2	1:A:411:LEU:CD1	2.29	0.62
1:D:143:LEU:O	1:D:147:ILE:HG22	1.99	0.62
1:D:332:PRO:HD2	1:D:459:LEU:HD13	1.80	0.61
1:B:318:PHE:HE1	1:C:317:ARG:HB3	1.66	0.61
1:D:251:PRO:O	1:D:255:LYS:HG3	2.01	0.61
1:D:144:PHE:HD2	1:D:197:LYS:HG2	1.66	0.60
1:B:153:LYS:CB	1:B:194:MET:HG2	2.30	0.60
1:B:524:LEU:HD23	1:B:525:CYS:SG	2.40	0.60
1:B:234:LEU:HD22	1:B:520:ASP:HB3	1.84	0.60
1:C:361:PHE:CZ	1:C:448:LEU:CD2	2.84	0.60
1:B:316:LEU:HD11	1:B:467:ASP:HA	1.82	0.60
1:C:224:PHE:O	1:C:228:THR:HG23	2.03	0.59
1:A:147:ILE:CD1	1:A:159:PHE:HA	2.31	0.59
1:C:140:GLU:CB	1:C:201:LYS:HG2	2.30	0.59
1:B:182:LEU:CD1	1:B:203:CYS:HB3	2.33	0.59
1:C:143:LEU:HD12	1:C:212:THR:HG23	1.85	0.59
1:C:196:ASP:OD1	1:C:197:LYS:N	2.36	0.59
1:B:153:LYS:HB3	1:B:194:MET:HG2	1.85	0.58
1:B:530:TYR:HH	1:C:461:HIS:HD1	1.50	0.58
1:C:157:HIS:CE1	1:C:158:LYS:HG3	2.39	0.58
2:B:601:QAJ:C4	1:D:321:LEU:HD23	2.33	0.57
1:B:479:PRO:HG3	1:C:530:TYR:CE1	2.39	0.57
1:D:379:GLN:HA	1:D:382:ARG:CD	2.35	0.57
1:B:143:LEU:HD22	1:B:200:PHE:HZ	1.70	0.57
1:D:234:LEU:HD22	1:D:520:ASP:HB3	1.84	0.57
1:A:141:ASP:HA	1:A:144:PHE:HB3	1.86	0.56
1:A:224:PHE:O	1:A:228:THR:HG23	2.05	0.56
1:C:281:PRO:HB3	1:C:370:TYR:HE1	1.71	0.56
1:A:317:ARG:HG3	1:D:325:GLU:OE2	2.06	0.56
1:C:293:TYR:OH	1:C:306:HIS:NE2	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:PHE:CD1	1:A:154:ILE:HD11	2.41	0.56
1:C:379:GLN:O	1:C:382:ARG:HG2	2.06	0.55
1:D:443:THR:HG1	1:D:445:GLU:HG2	1.67	0.55
1:A:318:PHE:HZ	1:D:317:ARG:HD3	1.71	0.55
1:C:195:LEU:HD11	1:C:199:LEU:HG	1.87	0.55
1:C:361:PHE:CD1	1:C:365:MET:CE	2.90	0.55
1:A:186:LEU:O	1:A:190:SER:HB3	2.07	0.55
1:A:488:ILE:HD12	1:A:514:GLY:HA3	1.88	0.55
1:B:227:PHE:O	1:B:231:ILE:HG12	2.05	0.55
1:A:318:PHE:HE2	1:D:317:ARG:HB2	1.70	0.55
1:A:343:SER:HA	1:A:410:ILE:HD12	1.88	0.55
1:B:195:LEU:HD12	1:B:199:LEU:HG	1.88	0.54
1:D:365:MET:HG3	1:D:447:VAL:HG11	1.88	0.54
1:A:318:PHE:CE2	1:D:317:ARG:HD3	2.42	0.54
1:C:253:LEU:HD22	1:C:485:ALA:HA	1.87	0.54
1:A:286:SER:HB3	1:A:289:LYS:NZ	2.23	0.54
1:B:318:PHE:HE1	1:C:317:ARG:CB	2.21	0.54
1:D:152:GLU:HG2	1:D:153:LYS:CD	2.34	0.54
1:D:250:ILE:HD11	1:D:253:LEU:HG	1.89	0.54
1:B:162:ALA:HB1	1:B:215:PHE:HE1	1.72	0.54
1:C:199:LEU:HD12	1:C:202:LYS:HG2	1.90	0.54
1:D:216:ARG:O	1:D:218:LYS:HG3	2.07	0.54
1:B:529:ASN:OD1	1:C:529:ASN:ND2	2.35	0.53
1:D:143:LEU:HD22	1:D:200:PHE:HZ	1.73	0.53
1:D:252:GLN:CB	1:D:377:THR:HG22	2.38	0.53
1:A:387:ARG:HA	1:A:390:ALA:HB3	1.91	0.53
1:A:411:LEU:HD12	1:A:411:LEU:H	1.73	0.53
1:B:318:PHE:CE1	1:C:317:ARG:CD	2.92	0.53
1:B:318:PHE:CE1	1:C:317:ARG:HD2	2.44	0.53
1:C:488:ILE:HD12	1:C:514:GLY:HA3	1.91	0.53
1:B:142:LEU:HD13	1:B:216:ARG:NH2	2.24	0.52
1:D:286:SER:HB3	1:D:289:LYS:NZ	2.24	0.52
1:A:140:GLU:OE1	1:A:140:GLU:N	2.42	0.52
1:A:195:LEU:HD12	1:A:199:LEU:HD23	1.91	0.52
1:D:151:GLN:HG3	1:D:152:GLU:H	1.74	0.52
1:D:349:VAL:O	1:D:354:LYS:HE3	2.09	0.52
1:D:147:ILE:HD11	1:D:159:PHE:HA	1.92	0.51
1:A:530:TYR:CE1	1:D:479:PRO:HG3	2.45	0.51
1:A:208:ILE:O	1:A:212:THR:HG23	2.09	0.51
1:C:481:LYS:HZ3	1:C:482:SER:H	1.57	0.51
1:A:300:LEU:HD13	1:A:304:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:PHE:HD2	1:A:475:HIS:CD2	2.28	0.51
1:C:427:ALA:HB3	1:C:499:MET:HG2	1.92	0.51
1:B:288:VAL:O	1:B:292:LYS:HG2	2.10	0.51
1:C:250:ILE:HG13	1:C:253:LEU:H	1.75	0.51
1:A:479:PRO:HG3	1:D:530:TYR:CE1	2.46	0.51
1:B:207:ASN:O	1:B:211:LEU:HD12	2.10	0.51
1:B:286:SER:HB3	1:B:289:LYS:NZ	2.26	0.51
1:D:182:LEU:O	1:D:186:LEU:HG	2.11	0.51
1:D:162:ALA:HB1	1:D:215:PHE:HE1	1.76	0.51
1:A:316:LEU:HD11	1:A:467:ASP:CB	2.41	0.51
1:C:162:ALA:HB1	1:C:215:PHE:HE1	1.74	0.51
1:D:207:ASN:HB2	1:D:211:LEU:CD1	2.41	0.51
1:C:199:LEU:HA	1:C:202:LYS:HB3	1.92	0.50
1:B:153:LYS:HB2	1:B:194:MET:HG2	1.93	0.50
1:B:529:ASN:CG	1:C:529:ASN:HD21	2.15	0.50
1:D:267:THR:HA	1:D:496:MET:HA	1.93	0.50
1:B:224:PHE:O	1:B:228:THR:HG23	2.11	0.50
1:A:274:SER:HB3	1:A:278:THR:HG21	1.92	0.50
1:B:143:LEU:HD22	1:B:200:PHE:CZ	2.47	0.50
1:B:337:GLY:O	1:B:341:VAL:HG23	2.11	0.50
1:B:143:LEU:CD2	1:B:147:ILE:HD11	2.42	0.50
1:C:249:TYR:CE1	1:C:484:VAL:HG21	2.46	0.50
2:B:601:QAJ:C7	1:D:321:LEU:HD22	2.42	0.50
1:C:204:VAL:HG23	1:C:208:ILE:HD13	1.93	0.50
1:C:235:TYR:CD2	1:C:236:GLU:HG2	2.47	0.49
1:C:532:ASN:HD22	1:C:535:HIS:H	1.60	0.49
1:D:439:PHE:CE2	1:D:446:ARG:HB2	2.47	0.49
1:B:201:LYS:O	1:B:205:GLN:HB2	2.12	0.49
1:D:251:PRO:HG2	1:D:252:GLN:HE22	1.76	0.49
1:C:143:LEU:O	1:C:147:ILE:HG13	2.12	0.49
1:D:370:TYR:HD2	1:D:423:THR:HG23	1.77	0.49
1:B:449:SER:O	1:B:453:VAL:HG23	2.13	0.49
1:C:143:LEU:CD2	1:C:147:ILE:HD11	2.43	0.49
1:C:251:PRO:HG2	1:C:252:GLN:NE2	2.28	0.49
1:B:164:LYS:NZ	1:B:169:ARG:HA	2.28	0.48
1:D:193:VAL:O	1:D:195:LEU:CD1	2.61	0.48
1:C:315:GLY:C	1:C:317:ARG:H	2.16	0.48
1:B:365:MET:HG3	1:B:447:VAL:HG11	1.95	0.48
1:D:207:ASN:HB2	1:D:211:LEU:HD11	1.95	0.48
1:A:316:LEU:HD11	1:A:467:ASP:OD1	2.12	0.48
1:A:156:VAL:HG13	1:A:193:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:ILE:HD12	1:C:252:GLN:HB2	1.95	0.48
1:C:250:ILE:CD1	1:C:253:LEU:HD12	2.43	0.48
1:D:286:SER:HB3	1:D:289:LYS:HZ2	1.79	0.48
1:C:281:PRO:HB3	1:C:370:TYR:CE1	2.49	0.48
1:A:359:MET:HE1	1:A:372:GLY:O	2.13	0.47
1:C:145:TYR:CE2	1:C:197:LYS:NZ	2.80	0.47
1:C:391:ILE:HG22	1:C:395:LEU:HD11	1.96	0.47
1:D:194:MET:C	1:D:195:LEU:HD12	2.34	0.47
1:B:316:LEU:HD21	1:B:467:ASP:O	2.13	0.47
1:D:453:VAL:O	1:D:457:LEU:HD12	2.15	0.47
1:B:358:VAL:O	1:B:362:LEU:HG	2.15	0.47
1:B:484:VAL:HA	1:B:505:LEU:HD11	1.97	0.47
1:D:199:LEU:O	1:D:202:LYS:HB3	2.14	0.47
1:A:318:PHE:N	1:A:318:PHE:CD1	2.82	0.47
1:B:435:ALA:HB2	1:B:491:VAL:HG13	1.96	0.46
1:A:140:GLU:HG2	1:A:201:LYS:HG2	1.96	0.46
1:A:286:SER:OG	1:A:466:TYR:OH	2.32	0.46
1:B:290:PRO:HD3	1:B:481:LYS:HD3	1.97	0.46
1:B:317:ARG:C	1:B:319:ASN:H	2.16	0.46
1:C:196:ASP:OD1	1:C:198:ASP:HB3	2.14	0.46
1:A:417:LEU:HD23	1:A:420:ILE:HD11	1.97	0.46
1:A:162:ALA:HB1	1:A:215:PHE:HE1	1.80	0.46
1:C:195:LEU:HD23	1:C:200:PHE:HA	1.98	0.46
1:C:361:PHE:CE1	1:C:447:VAL:HG12	2.48	0.46
1:D:152:GLU:HB3	1:D:153:LYS:H	1.15	0.46
1:D:411:LEU:HA	1:D:411:LEU:HD13	1.83	0.46
1:D:160:ILE:O	1:D:164:LYS:HG3	2.15	0.46
1:D:374:SER:OG	1:D:377:THR:HG23	2.16	0.46
1:B:477:GLY:O	1:B:529:ASN:HB2	2.15	0.45
1:C:382:ARG:NH2	1:C:412:ASP:OD2	2.48	0.45
1:A:290:PRO:HD3	1:A:481:LYS:HD3	1.98	0.45
1:B:153:LYS:HB2	1:B:194:MET:CE	2.46	0.45
1:B:260:LEU:HA	1:B:277:ASP:OD2	2.16	0.45
1:B:476:VAL:HG13	1:B:522:VAL:HG21	1.99	0.45
1:C:213:GLN:HB2	1:C:218:LYS:HB2	1.99	0.45
1:D:323:LEU:HD21	1:D:395:LEU:HD23	1.97	0.45
1:A:176:LYS:CE	1:A:180:ASP:OD2	2.65	0.45
1:A:293:TYR:OH	1:A:306:HIS:NE2	2.32	0.45
1:C:250:ILE:HG13	1:C:252:GLN:H	1.81	0.45
1:A:182:LEU:O	1:A:186:LEU:HD12	2.17	0.45
1:D:198:ASP:O	1:D:198:ASP:OD1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:SER:HB2	1:D:289:LYS:HD2	1.98	0.45
1:C:344:LEU:HA	1:C:347:GLN:HE21	1.82	0.45
1:C:450:PRO:HA	1:C:453:VAL:CG1	2.47	0.45
1:D:260:LEU:HD13	1:D:501:TRP:HH2	1.82	0.45
1:D:477:GLY:O	1:D:529:ASN:HB2	2.17	0.45
1:B:318:PHE:CD2	1:B:321:LEU:HD13	2.52	0.44
1:D:176:LYS:HE3	1:D:180:ASP:OD2	2.16	0.44
1:A:182:LEU:HD23	1:A:182:LEU:HA	1.86	0.44
1:C:138:SER:O	1:C:142:LEU:HG	2.18	0.44
1:C:184:LEU:HD23	1:C:184:LEU:HA	1.78	0.44
1:C:192:GLY:C	1:C:194:MET:H	2.21	0.44
1:D:391:ILE:HG22	1:D:395:LEU:HD11	1.99	0.44
1:B:177:GLU:H	1:B:177:GLU:CD	2.21	0.44
1:A:378:PHE:HE1	1:A:415:PHE:HB2	1.83	0.44
2:A:601:QAJ:C13	1:D:317:ARG:HD2	2.47	0.44
1:B:307:ARG:O	1:B:328:LYS:HE2	2.17	0.44
1:A:140:GLU:HB3	1:A:201:LYS:HB2	1.99	0.44
1:A:236:GLU:O	1:A:240:LYS:HD2	2.17	0.44
1:B:267:THR:HA	1:B:496:MET:HA	1.99	0.44
1:C:157:HIS:O	1:C:161:THR:HG23	2.17	0.44
1:C:295:ILE:HG12	1:C:361:PHE:CG	2.49	0.44
1:D:410:ILE:HA	1:D:410:ILE:HD13	1.82	0.44
1:D:285:GLN:CG	1:D:484:VAL:HG12	2.43	0.44
1:A:139:LEU:HG	1:A:212:THR:HG21	1.98	0.44
1:B:178:CYS:O	1:B:182:LEU:CD1	2.62	0.44
1:C:139:LEU:H	1:C:139:LEU:HD12	1.83	0.44
1:C:361:PHE:HE1	1:C:447:VAL:CG1	2.27	0.44
1:D:156:VAL:HG11	1:D:186:LEU:HD11	1.99	0.44
1:D:185:THR:HA	1:D:188:THR:OG1	2.18	0.44
1:B:141:ASP:N	1:B:141:ASP:OD1	2.51	0.43
1:B:349:VAL:CG1	1:B:353:GLU:HB2	2.49	0.43
1:D:224:PHE:O	1:D:228:THR:HG23	2.18	0.43
1:A:332:PRO:HD2	1:A:459:LEU:HD13	1.98	0.43
1:B:236:GLU:O	1:B:240:LYS:NZ	2.44	0.43
1:C:374:SER:OG	1:C:377:THR:HG23	2.18	0.43
1:C:239:LYS:HA	1:C:513:LYS:HD3	1.99	0.43
1:A:181:MET:O	1:A:185:THR:HG23	2.18	0.43
1:A:378:PHE:CE1	1:A:416:GLN:HG3	2.53	0.43
1:B:250:ILE:HD11	1:B:253:LEU:HD13	2.00	0.43
1:C:162:ALA:HB1	1:C:215:PHE:CE1	2.53	0.43
1:B:152:GLU:O	1:B:152:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:SER:HB3	1:A:289:LYS:HZ3	1.81	0.43
1:C:267:THR:HA	1:C:496:MET:HA	2.01	0.43
1:D:374:SER:HB2	1:D:421:GLU:OE2	2.17	0.43
1:A:253:LEU:HD21	1:A:285:GLN:HE21	1.83	0.43
1:B:299:ASP:OD2	1:B:357:TYR:OH	2.30	0.43
1:B:293:TYR:CE2	1:B:459:LEU:HD12	2.53	0.43
1:C:450:PRO:HA	1:C:453:VAL:HG12	1.99	0.43
1:D:147:ILE:O	1:D:158:LYS:NZ	2.35	0.43
1:A:137:PRO:O	1:A:138:SER:HB3	2.19	0.43
1:A:322:PHE:O	1:A:323:LEU:HD23	2.18	0.43
1:D:193:VAL:O	1:D:195:LEU:HD12	2.18	0.43
1:D:435:ALA:HB2	1:D:491:VAL:HG13	2.00	0.43
1:D:479:PRO:HD2	1:D:491:VAL:O	2.19	0.43
1:A:477:GLY:O	1:A:529:ASN:HB2	2.19	0.43
1:C:260:LEU:O	1:C:502:SER:HB2	2.19	0.43
1:D:227:PHE:O	1:D:231:ILE:HG12	2.19	0.43
1:D:422:VAL:HG21	1:D:427:ALA:HB2	2.00	0.43
1:D:332:PRO:CD	1:D:459:LEU:HD13	2.48	0.43
1:C:288:VAL:O	1:C:292:LYS:HG2	2.19	0.43
1:C:246:VAL:HG22	1:C:503:PRO:HB2	2.01	0.43
1:D:379:GLN:OE1	1:D:382:ARG:NH1	2.51	0.43
1:D:261:TRP:CE3	1:D:502:SER:HB2	2.54	0.42
1:B:278:THR:O	1:B:425:GLU:HG3	2.19	0.42
1:C:225:MET:HB3	1:C:225:MET:HE3	1.89	0.42
1:D:143:LEU:HD12	1:D:212:THR:HG22	2.00	0.42
1:A:267:THR:HG23	1:A:271:GLN:O	2.19	0.42
1:B:336:ALA:HA	1:B:391:ILE:HG21	2.01	0.42
1:B:423:THR:H	1:B:426:SER:HG	1.61	0.42
1:D:378:PHE:HZ	1:D:412:ASP:OD2	2.02	0.42
1:A:267:THR:HA	1:A:496:MET:HA	2.01	0.42
1:A:370:TYR:HD2	1:A:423:THR:HG23	1.83	0.42
1:C:286:SER:HB3	1:C:289:LYS:HZ3	1.84	0.42
1:C:333:MET:HG3	1:C:481:LYS:HD3	2.01	0.42
1:D:250:ILE:HD11	1:D:253:LEU:CG	2.49	0.42
1:A:144:PHE:HD2	1:A:145:TYR:CD1	2.36	0.42
1:A:261:TRP:HA	1:A:501:TRP:O	2.19	0.42
1:B:304:TYR:O	1:B:307:ARG:HB2	2.19	0.42
1:B:286:SER:OG	1:B:466:TYR:OH	2.31	0.42
1:C:252:GLN:N	1:C:252:GLN:OE1	2.52	0.42
1:C:272:ARG:HH12	1:C:369:GLU:CD	2.23	0.42
1:D:358:VAL:O	1:D:362:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:481:LYS:NZ	1:D:482:SER:O	2.53	0.42
1:B:162:ALA:HB1	1:B:215:PHE:CE1	2.54	0.42
1:C:358:VAL:HG11	1:C:417:LEU:HD22	2.01	0.42
1:D:359:MET:HB3	1:D:359:MET:HE2	1.83	0.42
1:B:199:LEU:HD12	1:B:199:LEU:HA	1.83	0.42
1:B:370:TYR:HD2	1:B:423:THR:HG23	1.84	0.42
1:C:143:LEU:HD12	1:C:212:THR:CG2	2.49	0.42
1:C:235:TYR:CE1	1:C:261:TRP:CD1	3.07	0.42
1:D:184:LEU:HA	1:D:184:LEU:HD12	1.77	0.42
1:D:480:ALA:HB2	1:D:490:LEU:HD12	2.01	0.42
1:B:365:MET:HB3	1:B:430:MET:HG2	2.01	0.42
1:C:250:ILE:CD1	1:C:252:GLN:HB2	2.50	0.42
1:D:285:GLN:O	1:D:288:VAL:HG12	2.20	0.42
1:D:427:ALA:HB3	1:D:499:MET:HG2	2.01	0.42
1:B:153:LYS:HB2	1:B:194:MET:HE2	2.01	0.42
1:A:317:ARG:HB2	1:D:318:PHE:CE2	2.54	0.41
1:B:486:GLY:O	1:B:501:TRP:HA	2.19	0.41
1:C:349:VAL:O	1:C:354:LYS:HE3	2.20	0.41
1:D:185:THR:O	1:D:188:THR:HB	2.20	0.41
1:D:322:PHE:O	1:D:323:LEU:HD23	2.20	0.41
1:C:249:TYR:HE1	1:C:484:VAL:HG21	1.83	0.41
1:B:140:GLU:CB	1:B:201:LYS:HG3	2.51	0.41
1:B:223:ASP:OD2	1:B:226:SER:OG	2.25	0.41
1:D:217:ARG:HE	1:D:217:ARG:HB2	1.81	0.41
1:C:176:LYS:HD3	1:C:180:ASP:OD2	2.20	0.41
1:C:155:PRO:HG3	1:C:194:MET:SD	2.61	0.41
1:D:271:GLN:HG3	1:D:271:GLN:H	1.61	0.41
1:D:293:TYR:OH	1:D:306:HIS:NE2	2.42	0.41
1:D:443:THR:OG1	1:D:445:GLU:CG	2.58	0.41
1:B:192:GLY:C	1:B:194:MET:H	2.24	0.41
1:B:530:TYR:CE1	1:C:479:PRO:HG3	2.55	0.41
1:D:147:ILE:HG12	1:D:154:ILE:HD13	2.01	0.41
1:D:156:VAL:HG21	1:D:186:LEU:HD11	2.02	0.41
1:B:143:LEU:O	1:B:143:LEU:HD23	2.21	0.41
1:D:151:GLN:CG	1:D:152:GLU:H	2.32	0.41
1:A:318:PHE:HZ	1:D:317:ARG:CD	2.32	0.41
1:B:474:PHE:HD2	1:B:475:HIS:CD2	2.38	0.41
1:A:143:LEU:HD23	1:A:143:LEU:O	2.20	0.41
1:B:502:SER:OG	1:B:504:PRO:HD2	2.20	0.41
1:C:365:MET:HG3	1:C:447:VAL:HG11	2.01	0.41
1:C:491:VAL:HG12	1:C:493:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:LEU:O	1:A:188:THR:HG23	2.21	0.41
1:A:387:ARG:O	1:A:391:ILE:N	2.31	0.41
1:B:295:ILE:HG23	1:B:361:PHE:CE2	2.56	0.41
1:C:228:THR:HB	1:C:273:HIS:CG	2.56	0.41
1:A:410:ILE:HD13	1:A:410:ILE:HA	1.92	0.41
1:B:228:THR:HB	1:B:273:HIS:CE1	2.56	0.41
1:D:162:ALA:HB1	1:D:215:PHE:CE1	2.56	0.41
1:A:324:ASN:HB3	1:A:330:HIS:ND1	2.36	0.40
1:D:281:PRO:HA	1:D:422:VAL:O	2.21	0.40
1:B:281:PRO:HA	1:B:422:VAL:O	2.21	0.40
1:B:318:PHE:CE1	1:C:317:ARG:CG	3.04	0.40
1:D:155:PRO:HG3	1:D:194:MET:SD	2.62	0.40
1:D:525:CYS:HA	1:D:540:LEU:O	2.20	0.40
1:B:140:GLU:HB3	1:B:201:LYS:HG3	2.04	0.40
1:B:185:THR:HA	1:B:188:THR:HB	2.02	0.40
1:B:289:LYS:HA	1:B:292:LYS:HE2	2.02	0.40
1:D:228:THR:HB	1:D:273:HIS:ND1	2.37	0.40
1:A:184:LEU:HD23	1:A:184:LEU:HA	1.84	0.40
1:A:286:SER:HB2	1:A:289:LYS:HD2	2.03	0.40
1:B:163:LEU:HD23	1:B:170:THR:HG22	2.03	0.40
1:D:318:PHE:CD1	1:D:321:LEU:HD12	2.56	0.40
1:B:302:THR:H	1:B:302:THR:HG23	1.70	0.40

All (10) 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:B:317:ARG:NH1	2:B:601:QAJ:N6[4_455]	1.27	0.93
1:C:317:ARG:NH1	2:B:601:QAJ:N10[4_455]	1.71	0.49
1:B:317:ARG:NH1	2:B:601:QAJ:C13[4_455]	1.79	0.41
1:C:317:ARG:NH1	2:B:601:QAJ:C23[4_455]	1.90	0.30
1:B:317:ARG:NH1	2:B:601:QAJ:C14[4_455]	1.91	0.29
1:B:255:LYS:NZ	1:D:189:THR:CG2[3_444]	1.92	0.28
1:B:317:ARG:CZ	2:B:601:QAJ:N6[4_455]	1.98	0.22
1:B:255:LYS:CE	1:D:189:THR:CG2[3_444]	2.06	0.14
1:A:387:ARG:N	1:C:397:GLU:OE1[4_555]	2.10	0.10
1:B:317:ARG:NE	2:B:601:QAJ:N6[4_455]	2.19	0.01

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%)	387 (95%)	19 (5%)	1 (0%)	47	78
1	B	408/527 (77%)	389 (95%)	18 (4%)	1 (0%)	47	78
1	C	408/527 (77%)	389 (95%)	18 (4%)	1 (0%)	47	78
1	D	408/527 (77%)	388 (95%)	17 (4%)	3 (1%)	22	54
All	All	1631/2108 (77%)	1553 (95%)	72 (4%)	6 (0%)	34	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	152	GLU
1	D	192	GLY
1	B	192	GLY
1	A	193	VAL
1	C	193	VAL
1	D	193	VAL

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	76
1	B	353/451 (78%)	341 (97%)	12 (3%)	37	71
1	C	353/451 (78%)	338 (96%)	15 (4%)	30	63
1	D	353/451 (78%)	345 (98%)	8 (2%)	50	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1412/1804 (78%)	1367 (97%)	45 (3%)	39 73

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	LYS
1	A	201	LYS
1	A	202	LYS
1	A	237	SER
1	A	319	ASN
1	A	361	PHE
1	A	374	SER
1	A	407	MET
1	A	446	ARG
1	A	524	LEU
1	B	141	ASP
1	B	217	ARG
1	B	245	LYS
1	B	317	ARG
1	B	343	SER
1	B	361	PHE
1	B	374	SER
1	B	382	ARG
1	B	387	ARG
1	B	398	LYS
1	B	412	ASP
1	B	524	LEU
1	C	151	GLN
1	C	187	GLN
1	C	194	MET
1	C	201	LYS
1	C	237	SER
1	C	319	ASN
1	C	333	MET
1	C	361	PHE
1	C	380	SER
1	C	382	ARG
1	C	384	SER
1	C	398	LYS
1	C	412	ASP
1	C	502	SER
1	C	507	LYS

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Mol	Chain	Res	Type
1	D	138	SER
1	D	178	CYS
1	D	201	LYS
1	D	237	SER
1	D	319	ASN
1	D	361	PHE
1	D	380	SER
1	D	412	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	C	347	GLN
1	C	532	ASN
1	D	187	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	QAJ	B	601	-	32,41,41	3.56	18 (56%)	35,55,55	3.31	19 (54%)
2	QAJ	A	601	-	32,41,41	2.43	8 (25%)	35,55,55	2.02	11 (31%)

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	B	601	-	-	5/16/34/34	0/5/5/5
2	QAJ	A	601	-	-	2/16/34/34	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	QAJ	C18-C19	-11.30	1.33	1.51
2	A	601	QAJ	C15-N1	8.39	1.45	1.32
2	B	601	QAJ	C21-C22	5.98	1.55	1.37
2	A	601	QAJ	C17-N9	5.55	1.47	1.35
2	B	601	QAJ	C7-N5	5.04	1.45	1.36
2	B	601	QAJ	C17-N9	4.93	1.46	1.35
2	B	601	QAJ	C16-N9	4.82	1.45	1.36
2	A	601	QAJ	C9-C10	-4.65	1.44	1.51
2	B	601	QAJ	C9-C8	4.58	1.62	1.51
2	B	601	QAJ	C8-N5	4.52	1.45	1.35
2	B	601	QAJ	C22-N10	4.12	1.45	1.33
2	B	601	QAJ	C23-N10	3.87	1.42	1.34
2	A	601	QAJ	C7-N5	3.64	1.43	1.36
2	B	601	QAJ	C2-N1	3.64	1.52	1.46
2	B	601	QAJ	C21-C20	3.60	1.46	1.38
2	B	601	QAJ	N4-N3	-3.51	1.30	1.37
2	A	601	QAJ	C16-N9	3.48	1.42	1.36
2	B	601	QAJ	C15-N1	3.12	1.37	1.32
2	A	601	QAJ	C8-N5	2.82	1.41	1.35
2	A	601	QAJ	C9-C8	-2.52	1.46	1.51
2	A	601	QAJ	N4-N3	-2.35	1.33	1.37
2	B	601	QAJ	O2-C17	-2.33	1.18	1.23
2	B	601	QAJ	C1-C2	2.17	1.58	1.52
2	B	601	QAJ	C18-C17	2.11	1.56	1.51
2	B	601	QAJ	C3-N1	-2.06	1.43	1.46
2	B	601	QAJ	C14-N6	-2.00	1.29	1.34

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	QAJ	C18-C17-N9	7.43	130.13	114.77
2	B	601	QAJ	C1-C5-C4	-7.42	97.96	110.82
2	A	601	QAJ	C1-C5-C4	-6.55	99.47	110.82
2	B	601	QAJ	C9-C8-N5	6.51	128.23	114.77
2	B	601	QAJ	O1-C8-N5	-4.99	114.52	123.63
2	B	601	QAJ	O2-C17-N9	-4.97	114.55	123.63
2	A	601	QAJ	C9-C8-N5	4.66	124.40	114.77
2	B	601	QAJ	C19-C18-C17	-4.48	99.30	112.57
2	B	601	QAJ	C20-C21-C22	4.42	125.45	118.91
2	B	601	QAJ	C1-C5-N2	4.23	117.19	110.60
2	B	601	QAJ	C18-C19-C23	-4.15	114.31	120.94
2	A	601	QAJ	C3-N1-C2	-4.13	102.39	111.52
2	A	601	QAJ	C18-C17-N9	3.90	122.82	114.77
2	B	601	QAJ	C6-N2-C5	-3.64	117.47	124.26
2	B	601	QAJ	C18-C19-C20	3.57	126.00	120.89
2	B	601	QAJ	C21-C22-N10	-3.30	113.11	122.58
2	B	601	QAJ	C9-C10-C11	3.21	125.48	120.89
2	B	601	QAJ	C3-N1-C2	-3.04	104.80	111.52
2	B	601	QAJ	O2-C17-C18	-2.95	115.32	122.03
2	B	601	QAJ	C19-C23-N10	2.94	129.46	123.72
2	B	601	QAJ	C21-C20-C19	-2.74	116.43	120.63
2	A	601	QAJ	O1-C8-C9	-2.67	115.95	122.03
2	B	601	QAJ	C7-N5-C8	-2.38	123.12	129.54
2	A	601	QAJ	C7-N5-C8	-2.35	123.20	129.54
2	A	601	QAJ	C16-N9-C17	-2.30	123.32	129.54
2	A	601	QAJ	O1-C8-N5	-2.21	119.59	123.63
2	B	601	QAJ	O1-C8-C9	-2.10	117.25	122.03
2	A	601	QAJ	C3-C4-C5	2.09	114.18	110.50
2	A	601	QAJ	O2-C17-C18	-2.07	117.32	122.03
2	A	601	QAJ	O2-C17-N9	-2.07	119.86	123.63

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	QAJ	S2-C15-N1-C2
2	B	601	QAJ	S2-C15-N1-C3
2	A	601	QAJ	S2-C15-N1-C3
2	A	601	QAJ	C4-C5-N2-C6
2	B	601	QAJ	C11-C10-C9-C8
2	B	601	QAJ	C4-C5-N2-C6

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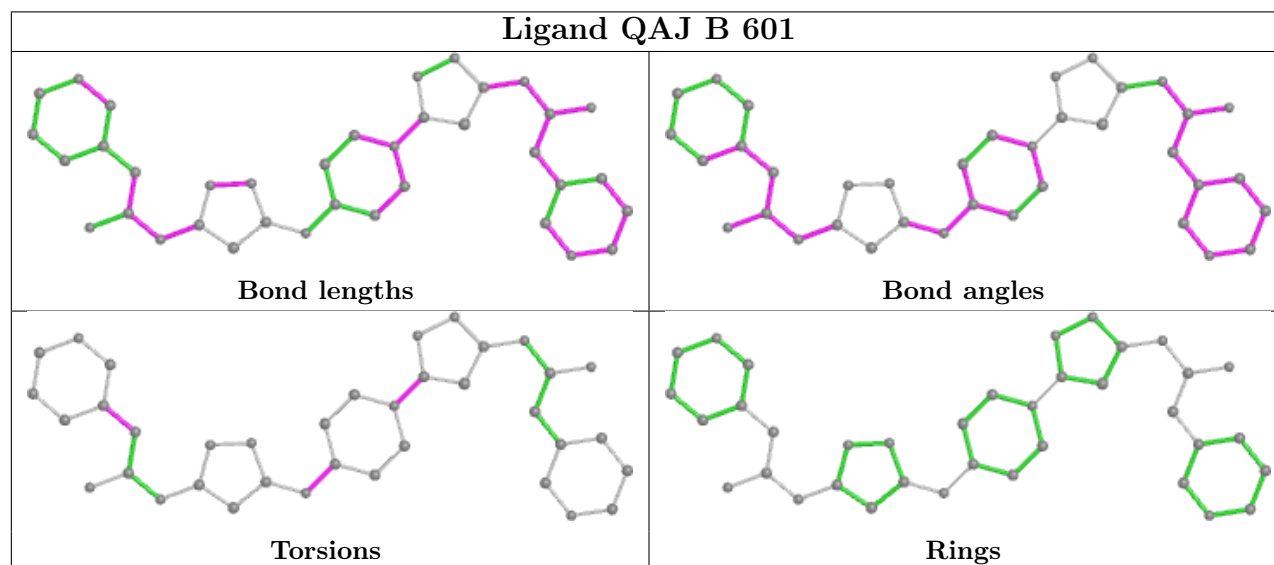
Mol	Chain	Res	Type	Atoms
2	B	601	QAJ	C14-C10-C9-C8

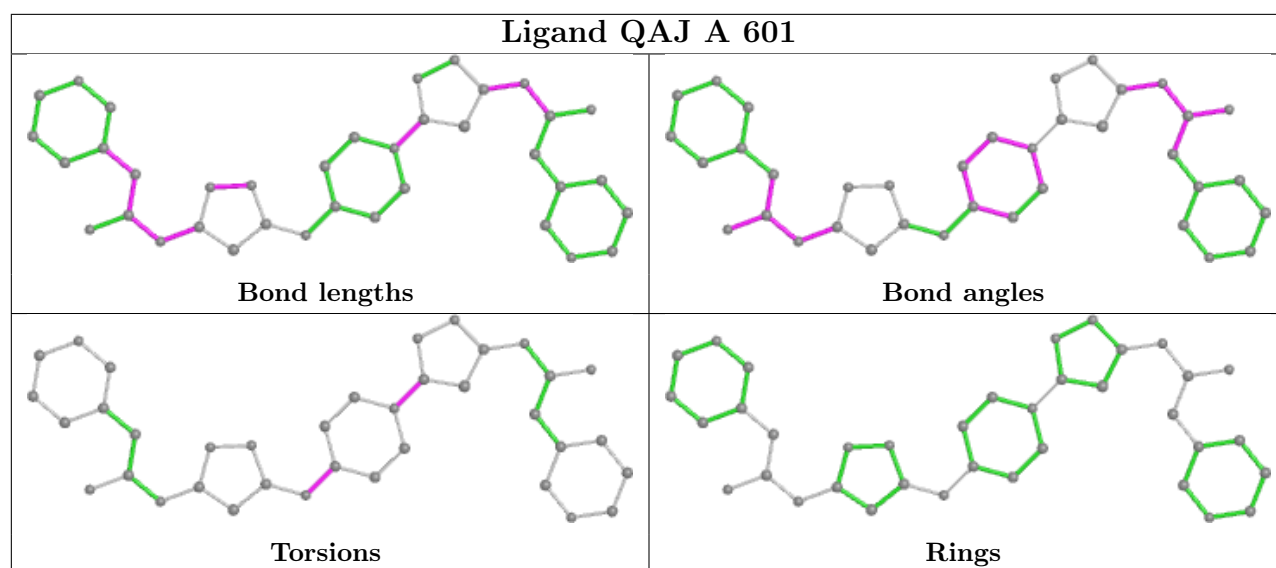
There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	QAJ	2	7
2	A	601	QAJ	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	409/527 (77%)	0.33	38 (9%) 8 6	44, 63, 120, 173	0
1	B	410/527 (77%)	0.44	40 (9%) 7 5	41, 64, 125, 187	0
1	C	410/527 (77%)	0.47	46 (11%) 5 4	41, 62, 125, 215	0
1	D	410/527 (77%)	0.36	36 (8%) 10 7	37, 62, 118, 185	0
All	All	1639/2108 (77%)	0.40	160 (9%) 7 5	37, 63, 122, 215	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	192	GLY	9.9
1	C	192	GLY	8.4
1	B	145	TYR	6.6
1	C	252	GLN	6.5
1	B	150	GLY	6.5
1	A	145	TYR	6.4
1	C	546	GLY	6.1
1	A	190	SER	5.8
1	C	250	ILE	5.7
1	A	138	SER	5.7
1	C	191	ASP	5.6
1	D	149	GLU	5.3
1	B	546	GLY	5.3
1	C	149	GLU	5.2
1	C	153	LYS	5.1
1	C	249	TYR	5.0
1	B	250	ILE	4.8
1	B	252	GLN	4.8
1	A	150	GLY	4.5
1	D	137	PRO	4.5
1	C	150	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	317	ARG	4.3
1	A	252	GLN	4.1
1	D	250	ILE	4.1
1	C	137	PRO	4.0
1	A	249	TYR	4.0
1	C	251	PRO	4.0
1	B	138	SER	4.0
1	B	191	ASP	3.9
1	D	546	GLY	3.9
1	C	348	GLY	3.7
1	C	197	LYS	3.6
1	A	144	PHE	3.6
1	D	249	TYR	3.6
1	B	153	LYS	3.6
1	A	151	GLN	3.6
1	D	318	PHE	3.5
1	D	251	PRO	3.4
1	C	253	LEU	3.4
1	B	249	TYR	3.4
1	A	137	PRO	3.4
1	C	152	GLU	3.4
1	C	545	GLU	3.4
1	A	348	GLY	3.4
1	B	149	GLU	3.3
1	C	145	TYR	3.3
1	D	141	ASP	3.2
1	C	287	CYS	3.2
1	B	144	PHE	3.2
1	A	316	LEU	3.2
1	C	489	LEU	3.2
1	D	252	GLN	3.2
1	A	152	GLU	3.2
1	B	152	GLU	3.2
1	A	317	ARG	3.1
1	B	180	ASP	3.1
1	A	352	ALA	3.1
1	D	383	GLU	3.1
1	B	545	GLU	3.1
1	B	489	LEU	3.1
1	D	152	GLU	3.0
1	B	148	ALA	3.0
1	C	384	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	191	ASP	3.0
1	A	489	LEU	2.9
1	C	205	GLN	2.9
1	B	176	LYS	2.9
1	D	145	TYR	2.9
1	B	348	GLY	2.9
1	A	498	MET	2.9
1	B	184	LEU	2.9
1	D	287	CYS	2.8
1	A	318	PHE	2.8
1	D	489	LEU	2.8
1	D	138	SER	2.7
1	A	148	ALA	2.7
1	B	251	PRO	2.7
1	D	189	THR	2.7
1	A	496	MET	2.7
1	D	317	ARG	2.6
1	C	512	VAL	2.6
1	A	188	THR	2.6
1	C	498	MET	2.6
1	C	198	ASP	2.6
1	B	510	ASN	2.6
1	C	148	ALA	2.6
1	D	142	LEU	2.6
1	C	193	VAL	2.6
1	B	151	GLN	2.6
1	A	142	LEU	2.6
1	B	490	LEU	2.6
1	B	253	LEU	2.5
1	C	325	GLU	2.5
1	C	180	ASP	2.5
1	C	279	LYS	2.5
1	B	287	CYS	2.5
1	A	250	ILE	2.5
1	D	490	LEU	2.5
1	A	222	PRO	2.5
1	D	291	LEU	2.5
1	D	498	MET	2.5
1	D	180	ASP	2.5
1	A	149	GLU	2.5
1	C	291	LEU	2.5
1	D	536	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	176	LYS	2.4
1	C	490	LEU	2.4
1	C	254	ALA	2.4
1	D	153	LYS	2.4
1	D	507	LYS	2.4
1	B	170	THR	2.4
1	D	196	ASP	2.4
1	C	511	SER	2.4
1	B	317	ARG	2.3
1	C	540	LEU	2.3
1	D	144	PHE	2.3
1	B	256	PHE	2.3
1	C	225	MET	2.3
1	A	200	PHE	2.3
1	A	287	CYS	2.3
1	C	188	THR	2.2
1	A	251	PRO	2.2
1	D	248	ASP	2.2
1	D	150	GLY	2.2
1	B	512	VAL	2.2
1	B	544	ARG	2.2
1	A	490	LEU	2.2
1	A	497	GLY	2.2
1	D	497	GLY	2.2
1	B	142	LEU	2.2
1	A	536	PHE	2.2
1	B	197	LYS	2.2
1	B	177	GLU	2.2
1	B	258	PRO	2.2
1	C	184	LEU	2.2
1	D	284	LEU	2.2
1	A	139	LEU	2.1
1	B	194	MET	2.1
1	C	144	PHE	2.1
1	C	318	PHE	2.1
1	D	538	LYS	2.1
1	A	141	ASP	2.1
1	A	380	SER	2.1
1	B	511	SER	2.1
1	C	284	LEU	2.1
1	A	349	VAL	2.1
1	A	291	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	356	ASP	2.1
1	A	387	ARG	2.1
1	B	325	GLU	2.1
1	B	349	VAL	2.1
1	C	245	LYS	2.0
1	A	177	GLU	2.0
1	D	348	GLY	2.0
1	B	275	THR	2.0
1	D	188	THR	2.0
1	C	213	GLN	2.0
1	C	491	VAL	2.0
1	C	508	MET	2.0
1	B	222	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 monosaccharides in this entry.

6.4 Ligands [i](#)

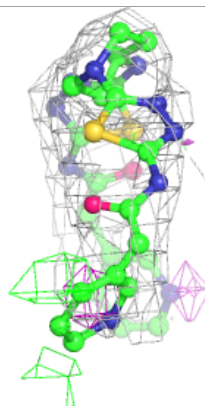
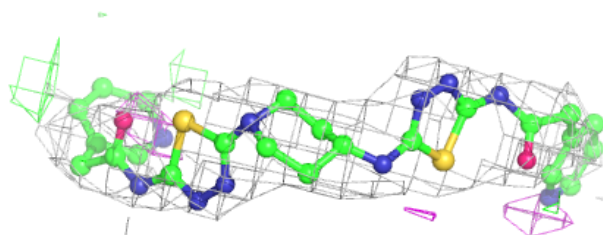
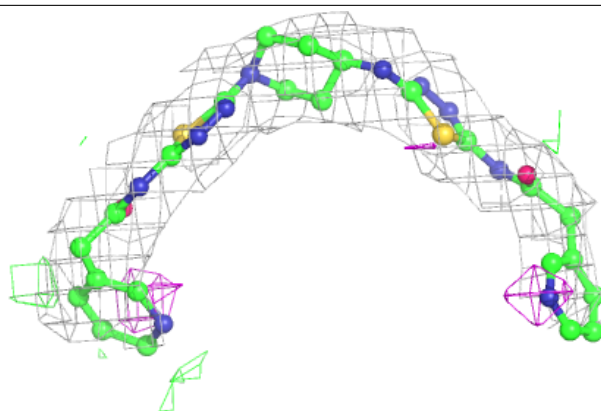
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	QAJ	B	601	37/37	0.90	0.27	55,77,176,192	0
2	QAJ	A	601	37/37	0.92	0.20	57,75,100,106	0

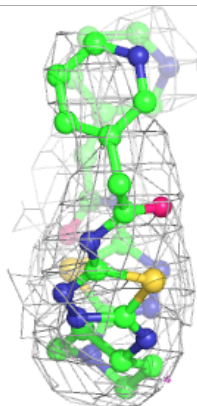
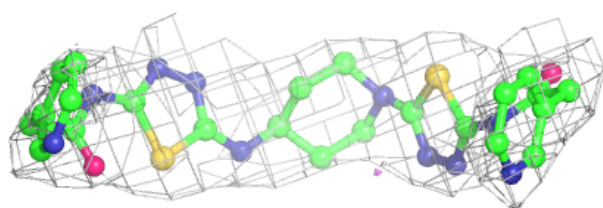
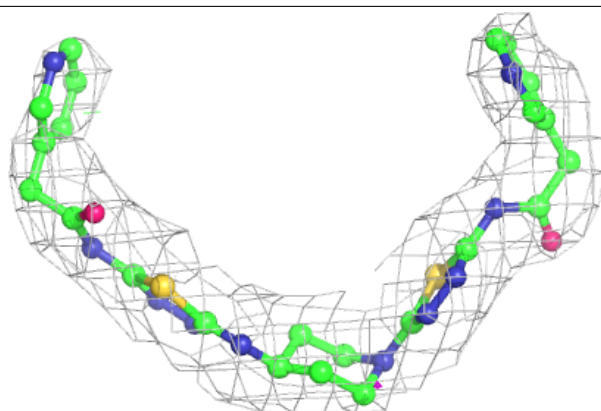
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

**Electron density around QAJ A 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.