



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:36 PM UTC

PDB ID : 6UME / pdb_00006ume
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 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

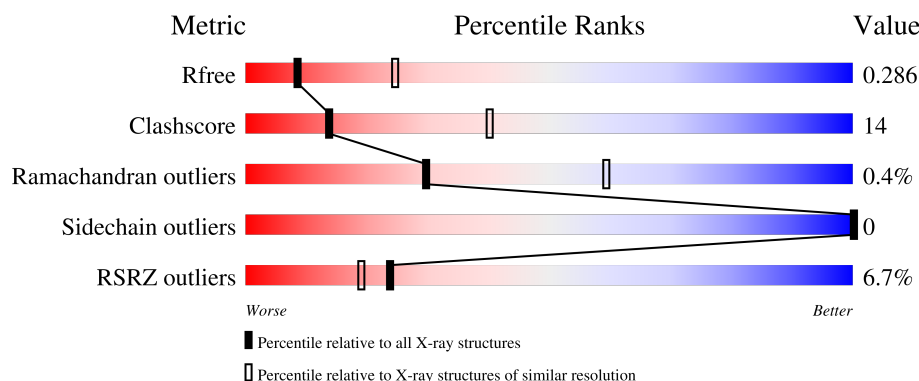
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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	5% 59% 17% • 22%
1	B	527	5% 55% 22% • 22%
1	C	527	5% 55% 22% • 22%
1	D	527	6% 54% 22% • 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	QAJ	B	601	-	X	-	-

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.

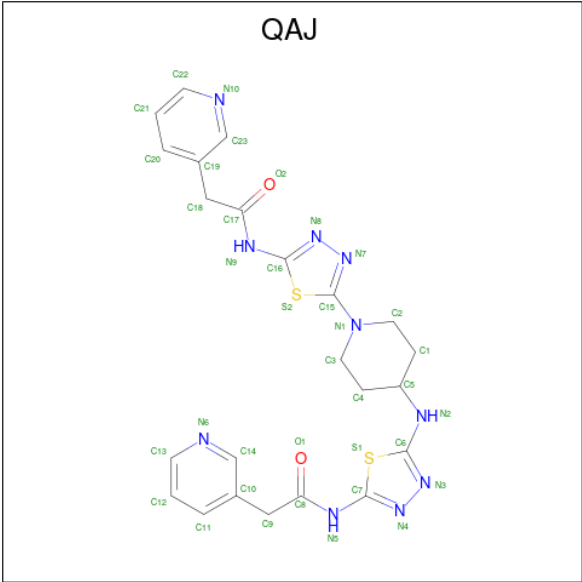
- Molecule 1 is a protein called Glutaminase kidney isoform, mitochondrial.

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 (CCD ID: QAJ) (formula: C₂₃H₂₄N₁₀O₂S₂) (labeled as "Ligand of Interest" by depositor).

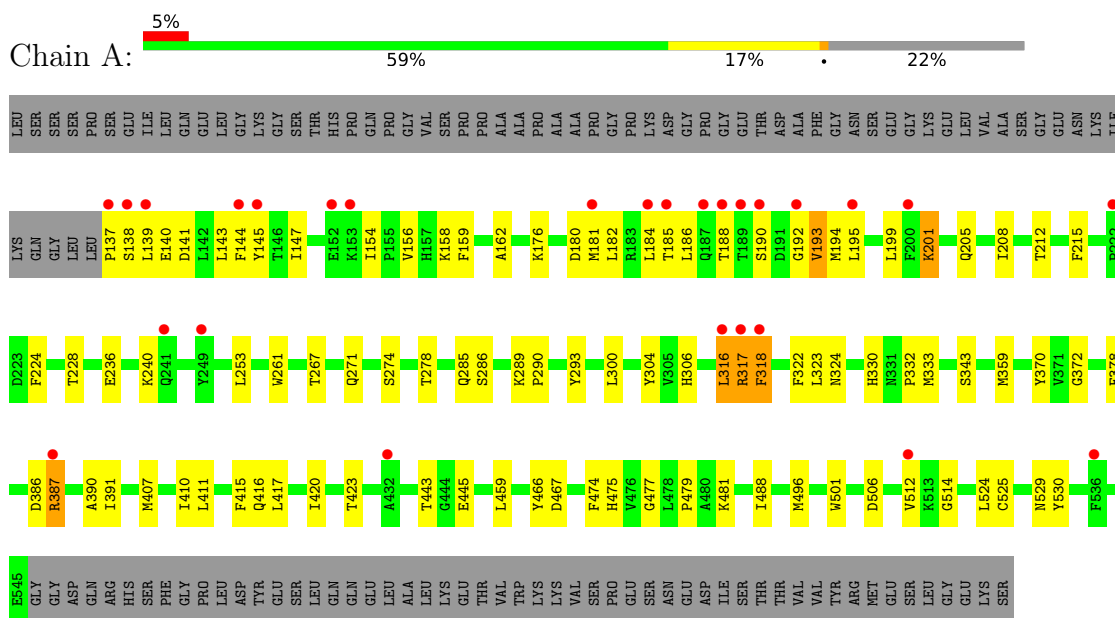


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			37	23	10	2	2		
2	B	1	Total	C	N	O	S	0	0
			37	23	10	2	2		

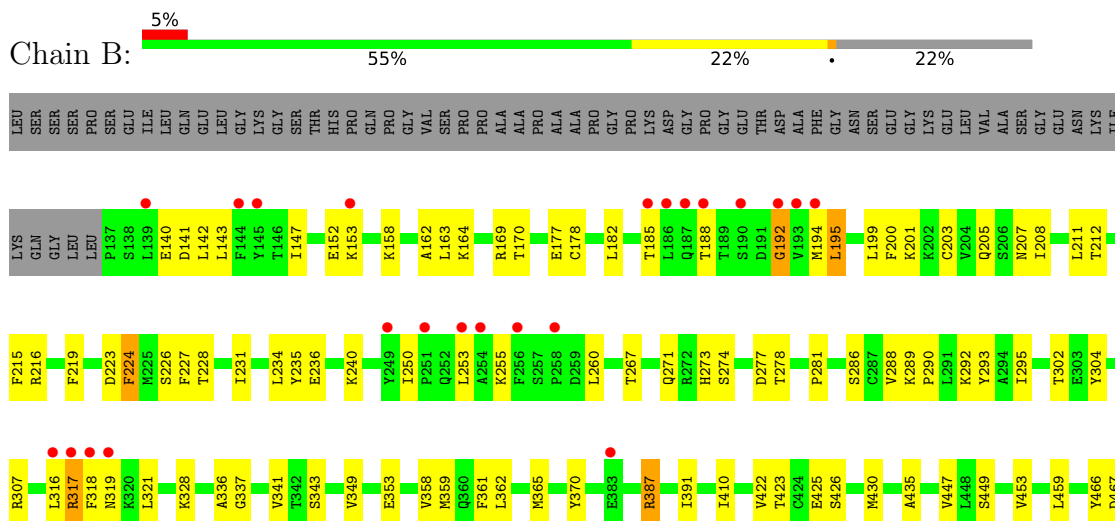
3 Residue-property plots

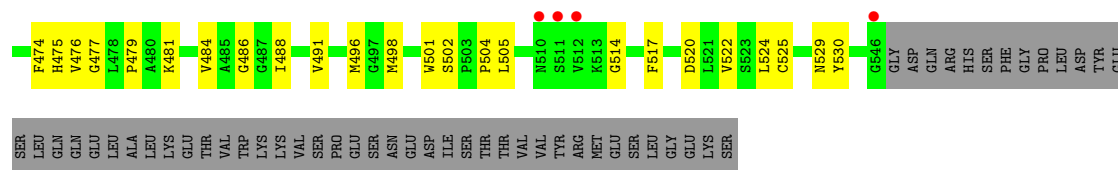
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

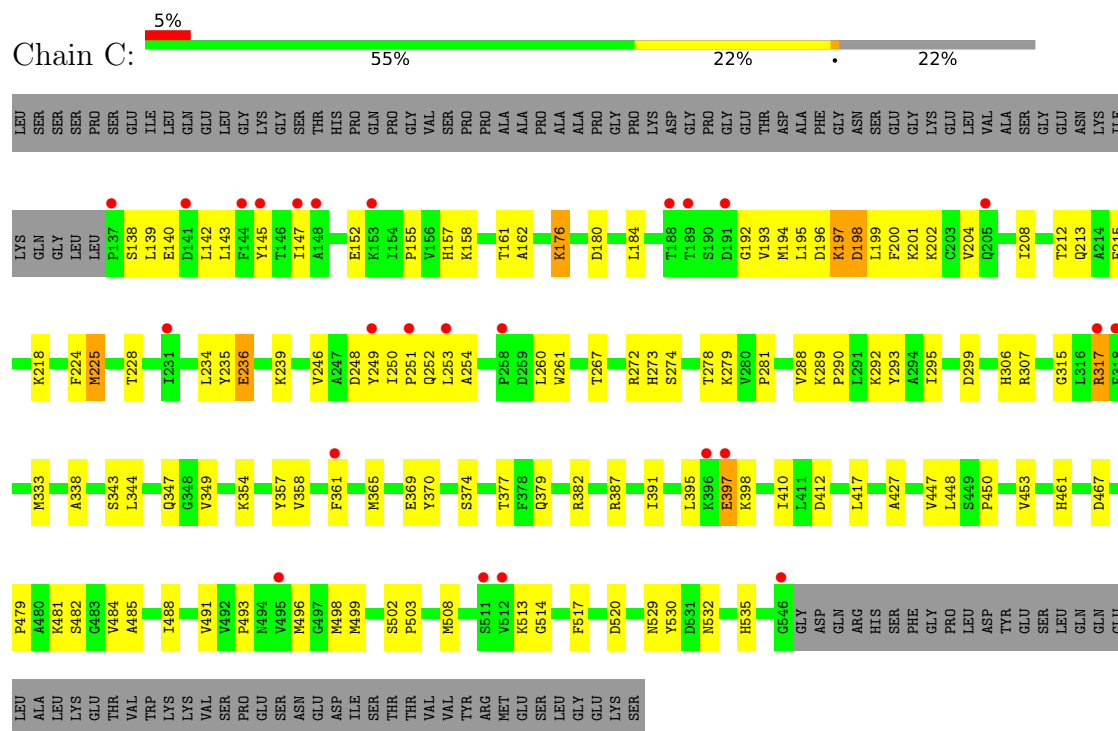


- Molecule 1: Glutaminase kidney isoform, mitochondrial

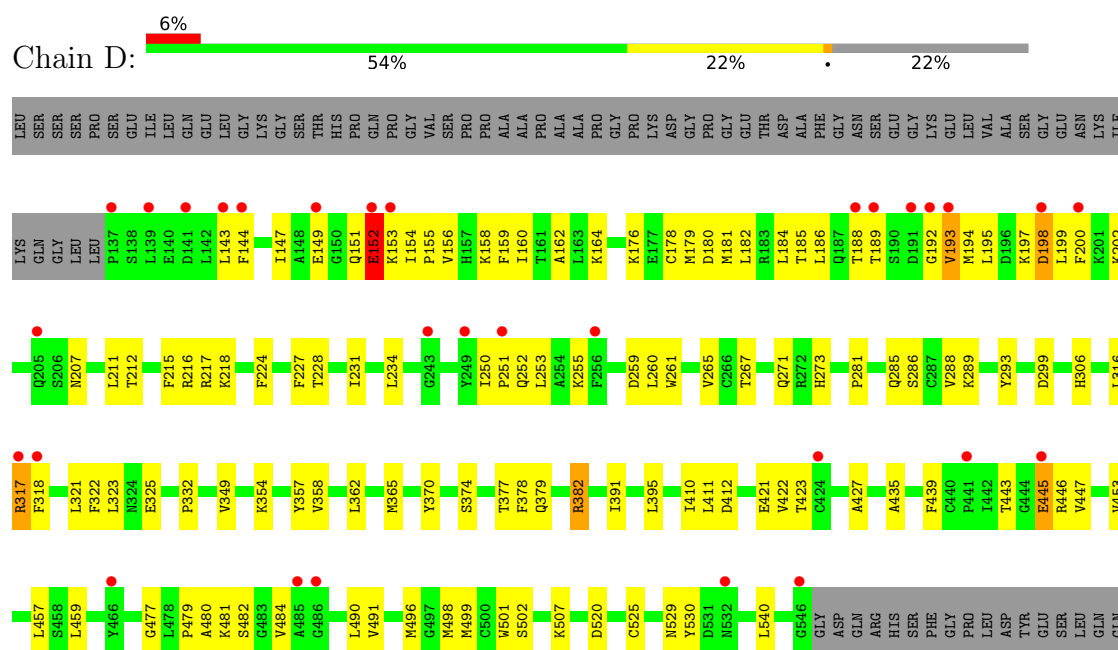




- Molecule 1: Glutaminase kidney isoform, mitochondrial



- Molecule 1: Glutaminase kidney isoform, mitochondrial



GLU
LEU
ALA
LEU
LYS
GLU
THR
VAL
LYS
LYS
VAL
SER
PRO
GLU
SER
ASN
GLU
ASP
ILE
SER
THR
THR
VAL
VAL
TYR
ARG
MET
GLU
SER
SER
LEU
GLY
GLU
LYS
SER

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) 99.0 (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)	Xtrriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.227 , 0.289 0.228 , 0.286	Depositor DCC
R_{free} test set	2000 reflections (3.16%)	wwPDB-VP
Wilson B-factor (Å ²)	57.9	Xtrriage
Anisotropy	0.985	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 66.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12846	wwPDB-VP
Average B, all atoms (Å ²)	71.0	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 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

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	0.50	2/3262 (0.1%)	0.80	4/4403 (0.1%)
1	B	0.44	1/3266 (0.0%)	0.76	5/4408 (0.1%)
1	C	0.52	1/3266 (0.0%)	0.92	13/4408 (0.3%)
1	D	0.46	1/3266 (0.0%)	0.84	7/4408 (0.2%)
All	All	0.48	5/13060 (0.0%)	0.83	29/17627 (0.2%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	ARG	CZ-NH2	-7.15	1.24	1.33
1	C	397	GLU	CB-CG	7.07	1.73	1.52
1	B	317	ARG	CZ-NH1	6.00	1.41	1.32
1	D	317	ARG	CB-CG	5.23	1.68	1.52
1	A	318	PHE	CB-CG	-5.03	1.39	1.50

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	197	LYS	CA-C-N	11.40	135.94	120.44
1	C	197	LYS	C-N-CA	11.40	135.94	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	149	GLU	CA-CB-CG	10.50	135.11	114.10
1	B	317	ARG	NE-CZ-NH1	-8.45	113.05	121.50
1	D	382	ARG	CB-CG-CD	8.15	130.06	111.30
1	C	152	GLU	CA-CB-CG	-7.51	99.09	114.10
1	C	236	GLU	CA-CB-CG	-7.47	99.15	114.10
1	A	201	LYS	CB-CG-CD	-7.15	94.86	111.30
1	D	152	GLU	CA-C-N	6.86	133.34	122.36
1	D	152	GLU	C-N-CA	6.86	133.34	122.36
1	C	397	GLU	CB-CG-CD	6.68	123.96	112.60
1	C	279	LYS	CA-CB-CG	6.53	127.16	114.10
1	D	507	LYS	CA-CB-CG	-6.46	101.17	114.10
1	C	176	LYS	CB-CA-C	-6.37	100.02	110.85
1	B	387	ARG	CG-CD-NE	6.26	125.78	112.00
1	C	198	ASP	N-CA-CB	-6.06	101.28	110.07
1	C	317	ARG	CG-CD-NE	-5.96	98.89	112.00
1	C	176	LYS	CA-CB-CG	-5.93	102.23	114.10
1	B	195	LEU	CA-CB-CG	5.82	136.68	116.30
1	C	398	LYS	CB-CG-CD	5.55	124.07	111.30
1	A	201	LYS	CG-CD-CE	5.53	124.03	111.30
1	C	387	ARG	CA-CB-CG	5.53	125.15	114.10
1	D	149	GLU	CB-CG-CD	5.50	121.95	112.60
1	C	225	MET	CA-CB-CG	5.39	124.89	114.10
1	A	317	ARG	N-CA-C	-5.34	106.81	113.38
1	D	198	ASP	CB-CA-C	5.32	118.97	109.29
1	A	316	LEU	CB-CG-CD2	-5.21	95.08	110.70
1	B	224	PHE	CA-C-N	-5.10	112.68	121.66
1	B	224	PHE	C-N-CA	-5.10	112.68	121.66

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	79	1
1	B	3194	0	3166	97	7
1	C	3194	0	3170	103	3
1	D	3194	0	3170	112	2
2	A	37	0	0	1	0
2	B	37	0	0	2	7
All	All	12846	0	12673	370	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 (370) 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	1.04
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
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:A:201:LYS:HD2	1:A:201:LYS:C	2.07	0.79
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: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:NZ	2.22	0.72
1:B:153:LYS:HB2	1:B:194:MET:HE2	1.73	0.71
1:C:145:TYR:OH	1:C:197:LYS:CE	2.38	0.71
1:D:285:GLN:HG3	1:D:484:VAL:HG12	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:TYR:CZ	1:C:197:LYS:NZ	2.59	0.70
1:C:361:PHE:CZ	1:C:448:LEU:HD23	2.27	0.69
1:A:147:ILE:O	1:A:158:LYS:NZ	2.22	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:290:PRO:HB3	1:C:333:MET:HE3	1.76	0.66
1:C:299:ASP:OD2	1:C:357:TYR:OH	2.09	0.66
1:B:236:GLU:HG3	1:B:240:LYS:HZ1	1.59	0.66
1:C:361:PHE:HE1	1:C:447:VAL:HG12	1.61	0.66
1:C:361:PHE:CD1	1:C:365:MET:HE2	2.31	0.65
1:B:208:ILE:O	1:B:212:THR:HG23	1.96	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: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
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:D:265:VAL:HG22	1:D:498:MET:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:361:PHE:CE1	1:C:365:MET:HE2	2.37	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:498:MET:HE1	1:B:517:PHE:CE1	2.39	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
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: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:529:ASN:CG	1:C:529:ASN:HD21	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:SER:HB3	1:A:289:LYS:NZ	2.23	0.54
1:D:178:CYS:SG	1:D:179:MET:HE2	2.48	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:C:315:GLY:C	1:C:317:ARG:H	2.16	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:N	1:A:140:GLU:OE1	2.42	0.52
1:C:481:LYS:HZ3	1:C:482:SER:H	1.56	0.52
1:A:195:LEU:HD12	1:A:199:LEU:HD23	1.91	0.52
1:A:293:TYR:OH	1:A:306:HIS:NE2	2.32	0.52
1:B:286:SER:HB3	1:B:289:LYS:HZ2	1.75	0.52
1:D:443:THR:HG1	1:D:445:GLU:HG2	1.70	0.52
1:D:151:GLN:HG3	1:D:152:GLU:H	1.74	0.52
1:D:194:MET:C	1:D:195:LEU:HD12	2.34	0.52
1:D:349:VAL:O	1:D:354:LYS:HE3	2.09	0.52
1:A:530:TYR:CE1	1:D:479:PRO:HG3	2.45	0.51
1:D:147:ILE:HD11	1:D:159:PHE:HA	1.92	0.51
1:A:208:ILE:O	1:A:212:THR:HG23	2.09	0.51
1:A:300:LEU:HD13	1:A:304:TYR:CE1	2.45	0.51
1:A:474:PHE:HD2	1:A:475:HIS:CD2	2.28	0.51
1:B:317:ARG:C	1:B:319:ASN:H	2.16	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:162:ALA:HB1	1:D:215:PHE:HE1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:LEU:O	1:D:186:LEU:HG	2.11	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: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:C:145:TYR:CE2	1:C:197:LYS:NZ	2.80	0.49
1:C:192:GLY:C	1:C:194:MET:H	2.21	0.49
1:D:251:PRO:HG2	1:D:252:GLN:HE22	1.76	0.49
1:D:496:MET:CE	1:D:498:MET:HE3	2.42	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:B:177:GLU:CD	1:B:177:GLU:H	2.21	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:467:ASP:HB2	1:C:508:MET:HE2	1.95	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
1:A:359:MET:HE1	1:A:372:GLY:O	2.12	0.48
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:C:498:MET:HE1	1:C:517:PHE:CE1	2.49	0.48
1:C:281:PRO:HB3	1:C:370:TYR:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:ILE:HG22	1:C:395:LEU:HD11	1.96	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:C:272:ARG:HH12	1:C:369:GLU:CD	2.23	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: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:HD13	1:D:411:LEU:HA	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:A:290:PRO:HA	1:A:333:MET:HE1	1.98	0.45
1:A:316:LEU:CD1	1:A:467:ASP:CG	2.74	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:B:192:GLY:C	1:B:194:MET:H	2.24	0.45
1:A:176:LYS:CE	1:A:180:ASP:OD2	2.65	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:OD1	1:D:198:ASP:O	2.35	0.45
1:D:286:SER:HB2	1:D:289:LYS:HD2	1.98	0.45
1:B:359:MET:HE3	1:B:359:MET:HB3	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:391:ILE:HG22	1:D:395:LEU:HD11	1.99	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:285:GLN:CG	1:D:484:VAL:HG12	2.43	0.44
1:D:410:ILE:HD13	1:D:410:ILE:HA	1.82	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:HD12	1:C:139:LEU:H	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:C:225:MET:HB3	1:C:225:MET:HE3	1.41	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:C:239:LYS:HA	1:C:513:LYS:HD3	1.99	0.43
1:C:374:SER:OG	1:C:377:THR:HG23	2.18	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:153:LYS:HB2	1:B:194:MET:CE	2.46	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
1:B:317:ARG:CD	1:B:317:ARG:C	2.92	0.43
1:C:267:THR:HA	1:C:496:MET:HA	2.01	0.43
1:D:181:MET:HE3	1:D:181:MET:HB2	1.82	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:293:TYR:CE2	1:B:459:LEU:HD12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:THR:H	1:B:426:SER:HG	1.61	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:192:GLY:C	1:A:194:MET:H	2.26	0.43
1:A:477:GLY:O	1:A:529:ASN:HB2	2.19	0.43
1:B:498:MET:HE2	1:B:498:MET:HB3	1.86	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:332:PRO:CD	1:D:459:LEU:HD13	2.48	0.43
1:D:422:VAL:HG21	1:D:427:ALA:HB2	2.00	0.43
1:C:246:VAL:HG22	1:C:503:PRO:HB2	2.01	0.43
1:C:288:VAL:O	1:C:292:LYS:HG2	2.19	0.43
1:D:252:GLN:CD	1:D:252:GLN:N	2.77	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: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: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: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:D:299:ASP:OD2	1:D:357:TYR:OH	2.37	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:286:SER:OG	1:B:466:TYR:OH	2.31	0.42
1:B:304:TYR:O	1:B:307:ARG:HB2	2.19	0.42
1:C:252:GLN:N	1:C:252:GLN:OE1	2.52	0.42
1:D:358:VAL:O	1:D:362:LEU:HG	2.19	0.42
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:D:184:LEU:HA	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: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:H	1:D:271:GLN:HG3	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: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:HD23	1:B:143:LEU:O	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: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:B:502:SER:OG	1:B:504:PRO:HD2	2.20	0.41
1:C:228:THR:HB	1:C:273:HIS:CG	2.56	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:PRO:HA	1:D:422:VAL:O	2.21	0.40
1:D:286:SER:HB3	1:D:289:LYS:HZ3	1.83	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:235:TYR:CD2	1:B:235:TYR:C	2.98	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%)	43	72
1	B	408/527 (77%)	389 (95%)	18 (4%)	1 (0%)	43	72
1	C	408/527 (77%)	389 (95%)	18 (4%)	1 (0%)	43	72
1	D	408/527 (77%)	388 (95%)	17 (4%)	3 (1%)	18	48
All	All	1631/2108 (77%)	1553 (95%)	72 (4%)	6 (0%)	30	59

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%)	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 (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	350	ASN
1	A	455	ASN
1	B	285	GLN
1	B	335	ASN
1	B	388	ASN
1	B	471	GLN
1	C	347	GLN
1	C	532	ASN
1	D	187	GLN
1	D	368	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	QAJ	B	601	-	41,41,41	3.66	24 (58%)	51,55,55	4.41	35 (68%)
2	QAJ	A	601	-	41,41,41	2.56	17 (41%)	51,55,55	3.72	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	B	601	-	-	10/24/34/34	0/5/5/5
2	QAJ	A	601	-	-	6/24/34/34	0/5/5/5

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	QAJ	C18-C19	-11.42	1.33	1.51
2	B	601	QAJ	C16-S2	7.87	1.87	1.73
2	B	601	QAJ	C21-C22	6.19	1.55	1.37
2	A	601	QAJ	C16-S2	6.06	1.84	1.73
2	A	601	QAJ	C7-S1	5.93	1.83	1.73
2	A	601	QAJ	C17-N9	5.81	1.47	1.37
2	B	601	QAJ	C17-N9	5.08	1.46	1.37
2	B	601	QAJ	C7-N5	4.93	1.45	1.38
2	A	601	QAJ	C15-N1	4.86	1.45	1.34
2	B	601	QAJ	C9-C8	4.82	1.62	1.52
2	B	601	QAJ	C7-S1	4.81	1.82	1.73
2	A	601	QAJ	C9-C10	-4.71	1.44	1.51
2	B	601	QAJ	C16-N9	4.67	1.45	1.38
2	B	601	QAJ	C8-N5	4.60	1.45	1.37
2	B	601	QAJ	C21-C20	4.44	1.46	1.38
2	B	601	QAJ	C22-N10	4.31	1.45	1.33
2	B	601	QAJ	N4-N3	-4.19	1.30	1.39
2	B	601	QAJ	C6-S1	4.16	1.80	1.73
2	B	601	QAJ	C23-N10	3.95	1.42	1.34
2	A	601	QAJ	C7-N5	3.30	1.43	1.38
2	A	601	QAJ	C6-S1	3.26	1.79	1.73
2	A	601	QAJ	C6-N3	3.17	1.35	1.31
2	A	601	QAJ	C16-N9	3.12	1.42	1.38
2	A	601	QAJ	N4-N3	-3.12	1.33	1.39
2	B	601	QAJ	C2-N1	3.01	1.52	1.47
2	A	601	QAJ	C16-N8	2.81	1.35	1.31
2	B	601	QAJ	C15-S2	2.74	1.81	1.75
2	A	601	QAJ	C15-S2	2.69	1.81	1.75
2	A	601	QAJ	C9-C8	-2.69	1.46	1.52
2	B	601	QAJ	C6-N3	2.67	1.35	1.31
2	B	601	QAJ	N8-N7	-2.66	1.34	1.39
2	A	601	QAJ	C8-N5	2.61	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	QAJ	O2-C17	-2.39	1.18	1.23
2	B	601	QAJ	C1-C2	2.24	1.58	1.52
2	A	601	QAJ	C7-N4	2.24	1.34	1.31
2	B	601	QAJ	C18-C17	2.21	1.56	1.52
2	B	601	QAJ	C5-N2	-2.21	1.42	1.46
2	B	601	QAJ	C16-N8	2.20	1.34	1.31
2	A	601	QAJ	C15-N7	2.17	1.35	1.31
2	A	601	QAJ	N8-N7	-2.11	1.35	1.39
2	B	601	QAJ	C14-N6	-2.04	1.29	1.34

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	QAJ	C18-C17-N9	12.90	130.13	114.40
2	A	601	QAJ	N9-C16-N8	12.26	131.76	120.81
2	B	601	QAJ	C9-C8-N5	11.34	128.23	114.40
2	B	601	QAJ	S2-C16-N8	-8.32	105.24	114.52
2	A	601	QAJ	C9-C8-N5	8.20	124.40	114.40
2	B	601	QAJ	N9-C16-N8	8.13	128.07	120.81
2	B	601	QAJ	C1-C5-C4	-7.44	97.96	110.80
2	A	601	QAJ	S2-C16-N8	-7.33	106.33	114.52
2	A	601	QAJ	N5-C7-N4	6.92	126.99	120.81
2	A	601	QAJ	C18-C17-N9	6.90	122.82	114.40
2	A	601	QAJ	C1-C5-C4	-6.56	99.47	110.80
2	B	601	QAJ	S1-C7-N4	-6.50	107.26	114.52
2	A	601	QAJ	C15-N7-N8	6.35	119.60	107.08
2	A	601	QAJ	S1-C7-N4	-6.21	107.59	114.52
2	B	601	QAJ	S1-C6-N3	-5.89	107.94	114.52
2	B	601	QAJ	C15-N7-N8	5.87	118.67	107.08
2	A	601	QAJ	S1-C6-N3	-5.42	108.47	114.52
2	A	601	QAJ	N1-C15-N7	5.32	127.19	116.91
2	B	601	QAJ	S2-C15-N1	5.19	127.25	120.31
2	B	601	QAJ	N5-C7-N4	5.17	125.43	120.81
2	A	601	QAJ	S2-C15-N1	5.11	127.15	120.31
2	A	601	QAJ	S2-C15-N7	-5.11	105.61	114.44
2	A	601	QAJ	C3-N1-C2	-5.05	102.38	112.68
2	B	601	QAJ	C7-N4-N3	5.01	118.39	112.02
2	B	601	QAJ	C16-N8-N7	4.90	118.26	112.02
2	B	601	QAJ	C18-C19-C23	-4.65	114.32	120.98
2	B	601	QAJ	C20-C21-C22	4.51	125.44	118.92
2	B	601	QAJ	C19-C18-C17	-4.37	99.29	112.33
2	B	601	QAJ	N1-C15-N7	4.24	125.10	116.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	QAJ	O1-C8-N5	-4.18	114.52	122.44
2	B	601	QAJ	O2-C17-N9	-4.16	114.55	122.44
2	A	601	QAJ	C7-N4-N3	4.02	117.13	112.02
2	A	601	QAJ	C6-N3-N4	4.01	117.12	112.02
2	B	601	QAJ	C5-N2-C6	-3.99	117.47	124.48
2	B	601	QAJ	S2-C15-N7	-3.93	107.63	114.44
2	B	601	QAJ	C3-N1-C2	-3.87	104.80	112.68
2	B	601	QAJ	C6-N3-N4	3.82	116.89	112.02
2	A	601	QAJ	C16-N8-N7	3.58	116.57	112.02
2	B	601	QAJ	C18-C19-C20	3.47	126.00	120.89
2	B	601	QAJ	C21-C22-N10	-3.39	113.11	122.61
2	B	601	QAJ	C1-C5-N2	3.31	117.19	110.57
2	B	601	QAJ	C9-C10-C11	3.13	125.48	120.89
2	B	601	QAJ	O2-C17-C18	-3.08	115.32	121.99
2	B	601	QAJ	C19-C23-N10	2.99	129.46	123.75
2	B	601	QAJ	C21-C20-C19	-2.97	116.44	120.61
2	A	601	QAJ	O1-C8-C9	-2.79	115.95	121.99
2	B	601	QAJ	S1-C7-N5	2.61	127.21	123.72
2	B	601	QAJ	C1-C2-N1	2.27	115.11	110.66
2	B	601	QAJ	C17-N9-C16	2.22	127.49	123.69
2	A	601	QAJ	C3-C4-C5	2.22	114.18	110.67
2	B	601	QAJ	S2-C16-N9	2.21	126.68	123.72
2	B	601	QAJ	O1-C8-C9	-2.19	117.25	121.99
2	A	601	QAJ	O2-C17-C18	-2.16	117.32	121.99
2	B	601	QAJ	C2-N1-C15	-2.11	116.75	122.09

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	QAJ	S2-C15-N1-C3
2	A	601	QAJ	S2-C16-N9-C17
2	B	601	QAJ	N7-C15-N1-C3
2	B	601	QAJ	S2-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	C14-C10-C9-C8
2	A	601	QAJ	C4-C5-N2-C6
2	A	601	QAJ	N7-C15-N1-C3
2	B	601	QAJ	S1-C7-N5-C8
2	A	601	QAJ	N8-C16-N9-C17

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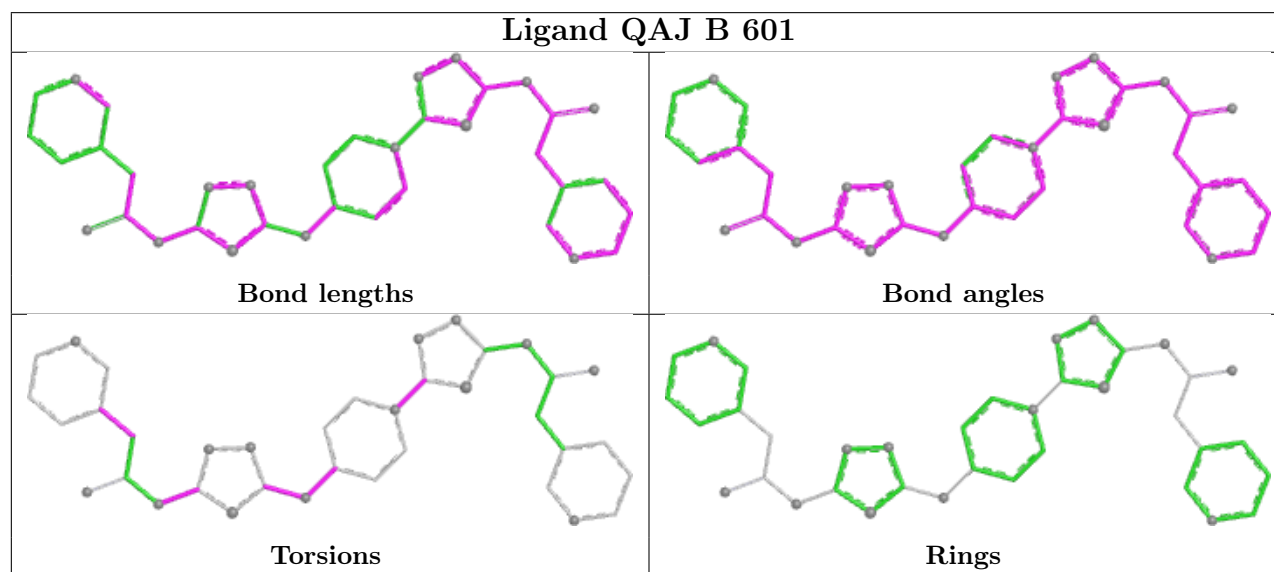
Mol	Chain	Res	Type	Atoms
2	B	601	QAJ	C4-C5-N2-C6
2	B	601	QAJ	C11-C10-C9-C8
2	B	601	QAJ	N7-C15-N1-C2
2	A	601	QAJ	O2-C17-C18-C19

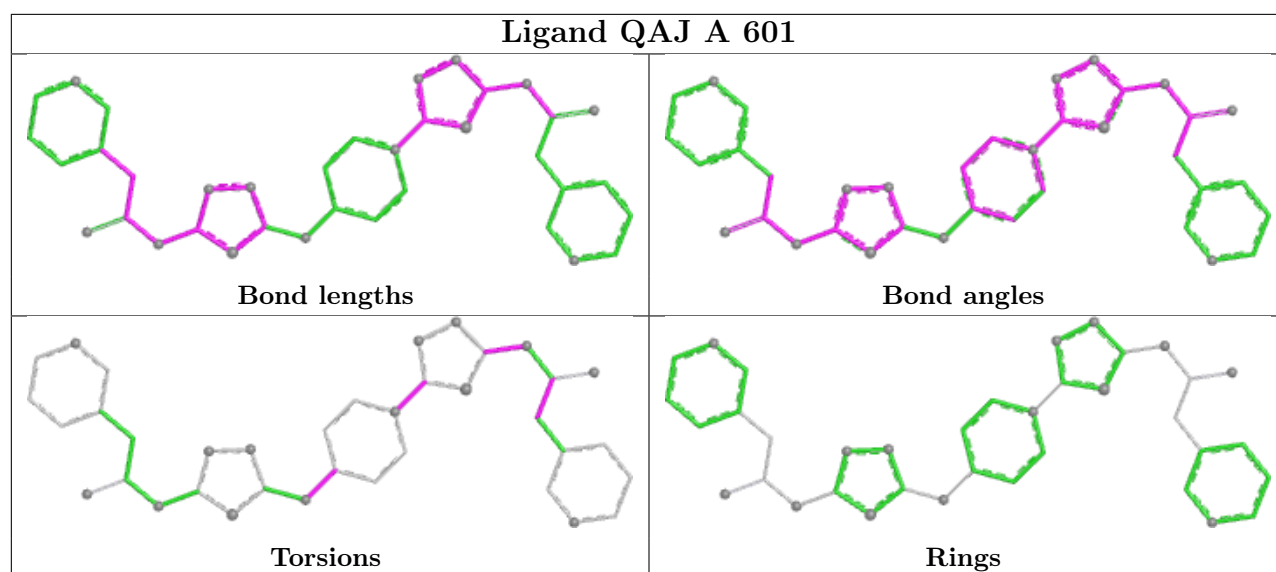
There are no ring outliers.

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%)	0.44	27 (6%) 24 19	44, 63, 120, 173	0
1	B	410/527 (77%)	0.51	27 (6%) 24 19	41, 64, 125, 187	0
1	C	410/527 (77%)	0.45	25 (6%) 27 21	41, 62, 125, 215	0
1	D	410/527 (77%)	0.45	30 (7%) 21 17	37, 62, 118, 185	0
All	All	1639/2108 (77%)	0.46	109 (6%) 24 19	37, 63, 122, 215	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	145	TYR	5.2
1	A	144	PHE	4.6
1	A	317	ARG	4.5
1	D	318	PHE	4.5
1	B	511	SER	4.1
1	A	188	THR	4.0
1	A	200	PHE	3.9
1	A	241	GLN	3.9
1	D	188	THR	3.9
1	C	188	THR	3.8
1	C	317	ARG	3.7
1	C	253	LEU	3.7
1	B	319	ASN	3.7
1	A	318	PHE	3.7
1	D	193	VAL	3.6
1	B	144	PHE	3.6
1	A	316	LEU	3.4
1	C	397	GLU	3.4
1	A	185	THR	3.4
1	A	190	SER	3.4
1	A	153	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	189	THR	3.3
1	B	318	PHE	3.3
1	C	318	PHE	3.2
1	D	424	CYS	3.1
1	D	532	ASN	3.1
1	A	387	ARG	3.1
1	B	316	LEU	3.1
1	D	189	THR	3.1
1	C	148	ALA	3.0
1	B	249	TYR	3.0
1	D	317	ARG	3.0
1	B	193	VAL	3.0
1	C	396	LYS	3.0
1	A	138	SER	3.0
1	A	139	LEU	2.9
1	B	145	TYR	2.9
1	C	546	GLY	2.9
1	D	205	GLN	2.9
1	C	137	PRO	2.9
1	A	249	TYR	2.9
1	C	145	TYR	2.9
1	D	153	LYS	2.8
1	D	198	ASP	2.8
1	B	256	PHE	2.8
1	D	200	PHE	2.8
1	B	188	THR	2.7
1	B	253	LEU	2.7
1	C	361	PHE	2.6
1	D	192	GLY	2.6
1	B	185	THR	2.6
1	B	546	GLY	2.6
1	D	486	GLY	2.6
1	A	432	ALA	2.6
1	C	141	ASP	2.6
1	A	187	GLN	2.6
1	C	205	GLN	2.5
1	D	149	GLU	2.5
1	B	510	ASN	2.5
1	D	143	LEU	2.4
1	D	139	LEU	2.4
1	C	147	ILE	2.4
1	B	317	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	251	PRO	2.4
1	C	153	LYS	2.4
1	B	139	LEU	2.4
1	D	441	PRO	2.4
1	C	512	VAL	2.3
1	B	192	GLY	2.3
1	A	536	PHE	2.3
1	B	187	GLN	2.3
1	A	137	PRO	2.3
1	B	153	LYS	2.3
1	A	184	LEU	2.3
1	D	249	TYR	2.3
1	A	512	VAL	2.3
1	D	546	GLY	2.3
1	D	256	PHE	2.3
1	B	254	ALA	2.3
1	C	191	ASP	2.3
1	C	249	TYR	2.2
1	A	181	MET	2.2
1	D	191	ASP	2.2
1	C	258	PRO	2.2
1	D	144	PHE	2.2
1	B	186	LEU	2.2
1	A	222	PRO	2.2
1	A	192	GLY	2.2
1	A	195	LEU	2.2
1	A	152	GLU	2.2
1	B	194	MET	2.2
1	D	137	PRO	2.1
1	C	144	PHE	2.1
1	B	190	SER	2.1
1	D	445	GLU	2.1
1	B	258	PRO	2.1
1	D	141	ASP	2.1
1	D	466	TYR	2.1
1	D	485	ALA	2.1
1	D	152	GLU	2.1
1	D	243	GLY	2.1
1	C	511	SER	2.1
1	B	512	VAL	2.1
1	C	231	ILE	2.1
1	B	383	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	495	VAL	2.0
1	D	251	PRO	2.0
1	A	189	THR	2.0
1	B	251	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](#)

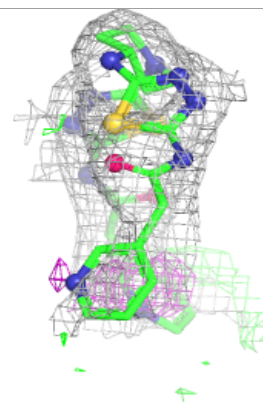
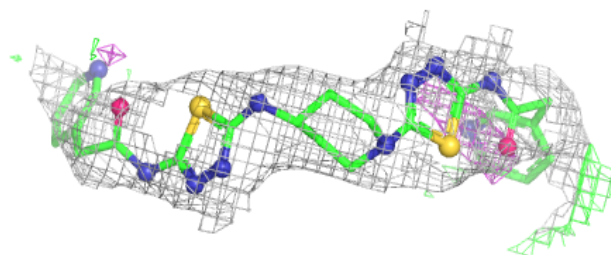
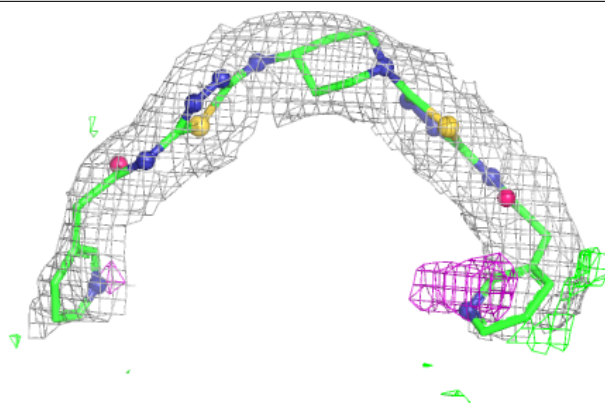
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	QAJ	B	601	37/37	0.89	0.14	55,77,176,192	0
2	QAJ	A	601	37/37	0.92	0.12	57,75,100,106	0

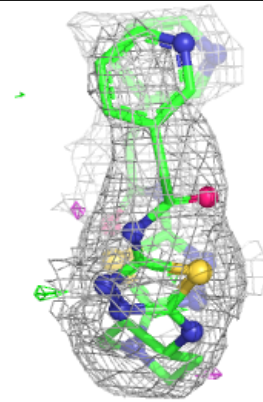
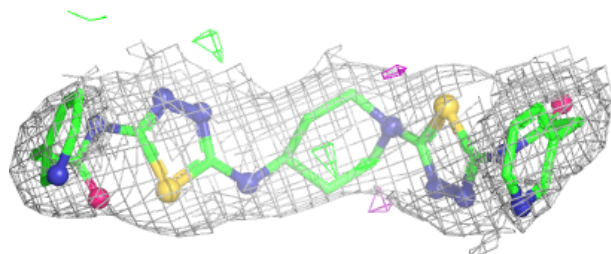
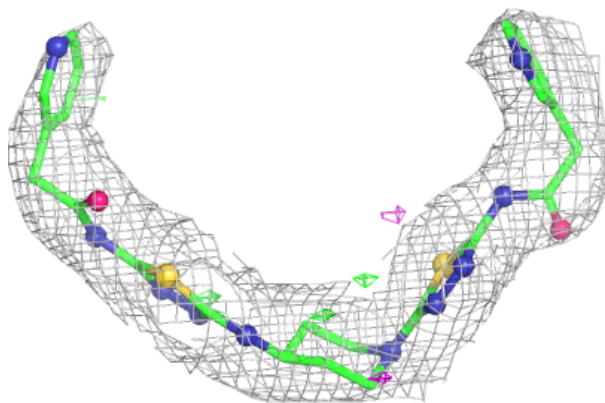
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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