



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:32 AM UTC

PDB ID : 6UMC / pdb_00006umc
Title : Crystal structure of human GAC in complex with inhibitor UPGL00012
Authors : Huang, Q.; Cerione, R.A.
Deposited on : 2019-10-09
Resolution : 2.75 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

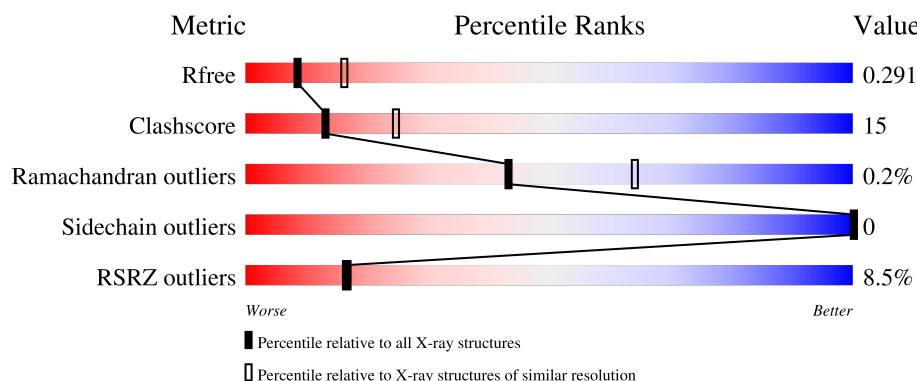
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	527	7% 57% 19% • 22%
1	B	527	8% 53% 23% • 22%
1	C	527	7% 53% 24% • 22%
1	D	527	6% 57% 20% • 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	U27	B	601	-	X	-	-
2	U27	C	601	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12881 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.

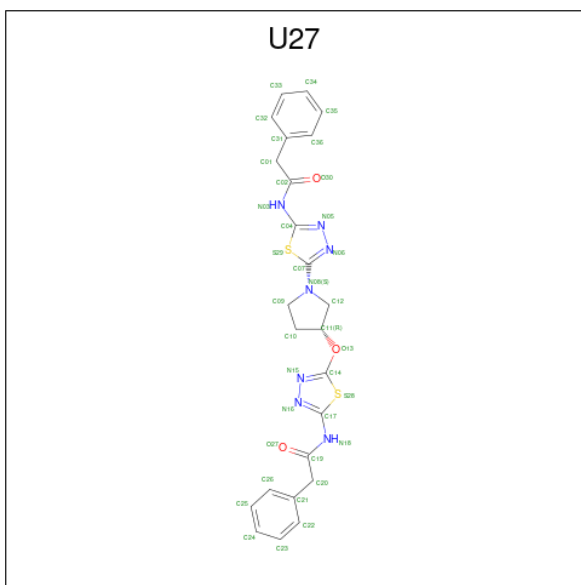
- Molecule 1 is a protein called Glutaminase kidney isoform, mitochondrial.

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-phenyl-N-{5-[(3R)-3-({5-[(phenylacetyl)amino]-1,3,4-thiadiazol-2-yl}oxy)pyrrolidin-1-yl]-1,3,4-thiadiazol-2-yl}acetamide (CCD ID: U27) (formula: C₂₄H₂₃N₇O₃S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total 36	C 24	N 7	O 3	S 2	0	0
2	C	1	Total 36	C 24	N 7	O 3	S 2	0	0

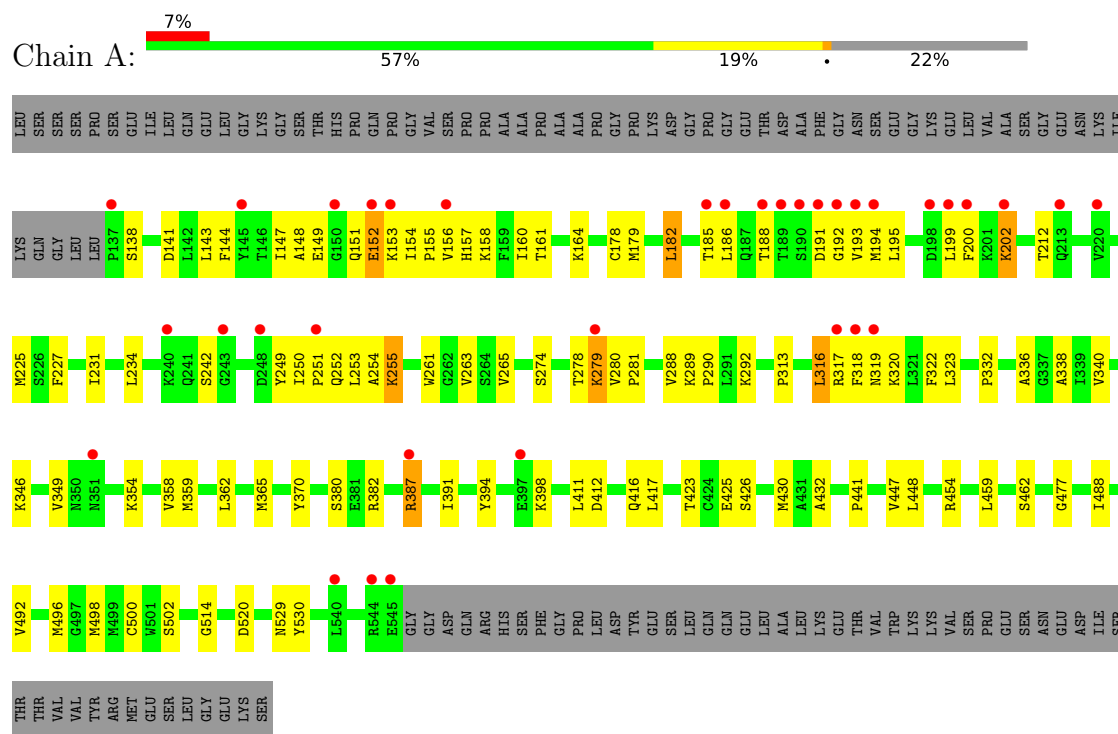
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	9	Total O 9 9	0	0
3	B	11	Total O 11 11	0	0
3	C	8	Total O 8 8	0	0
3	D	9	Total O 9 9	0	0

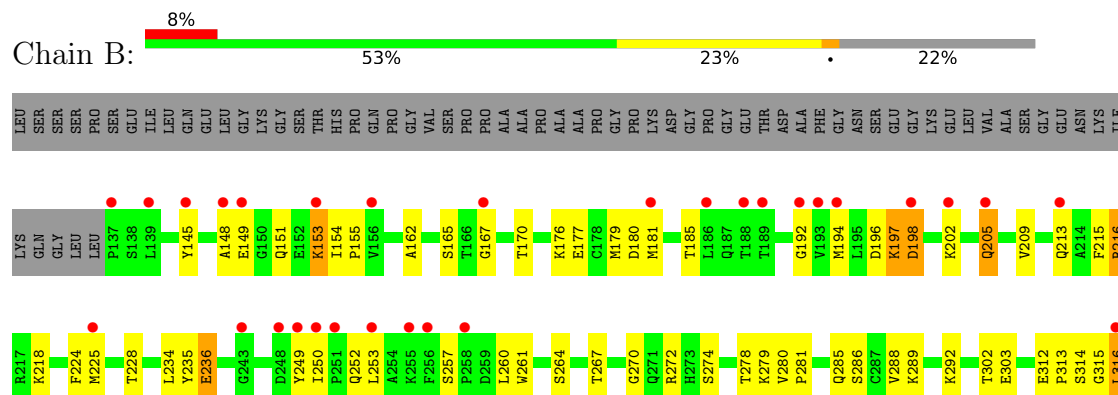
3 Residue-property plots

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

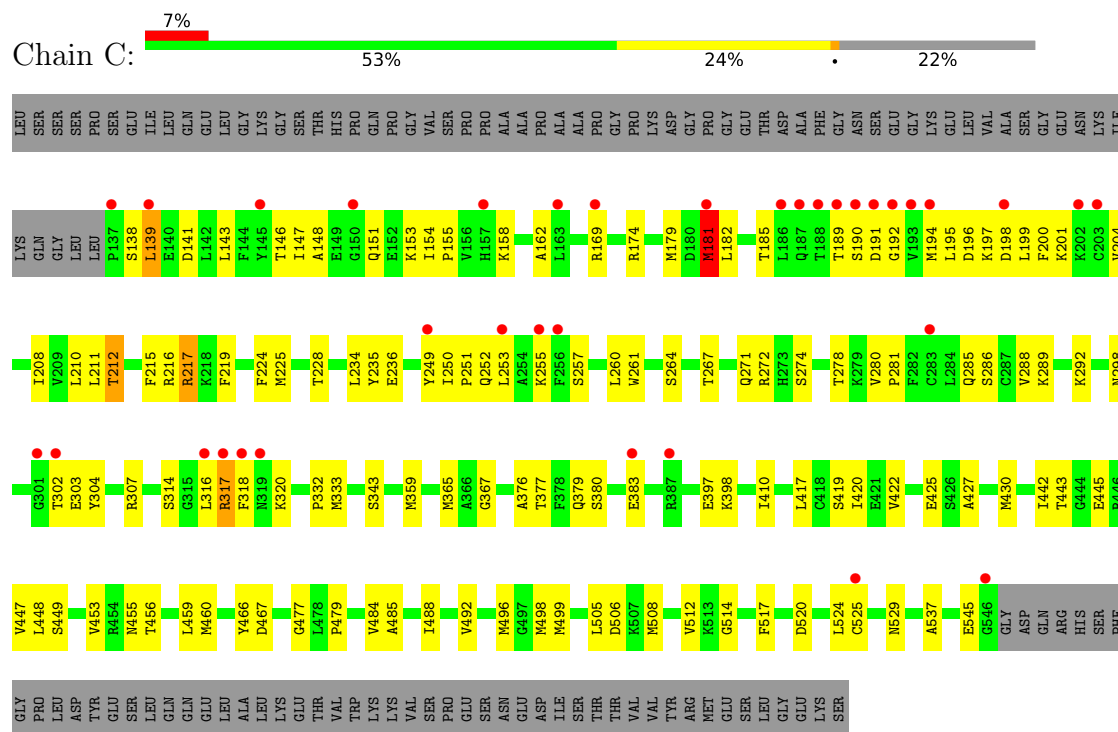
- Molecule 1: Glutaminase kidney isoform, mitochondrial



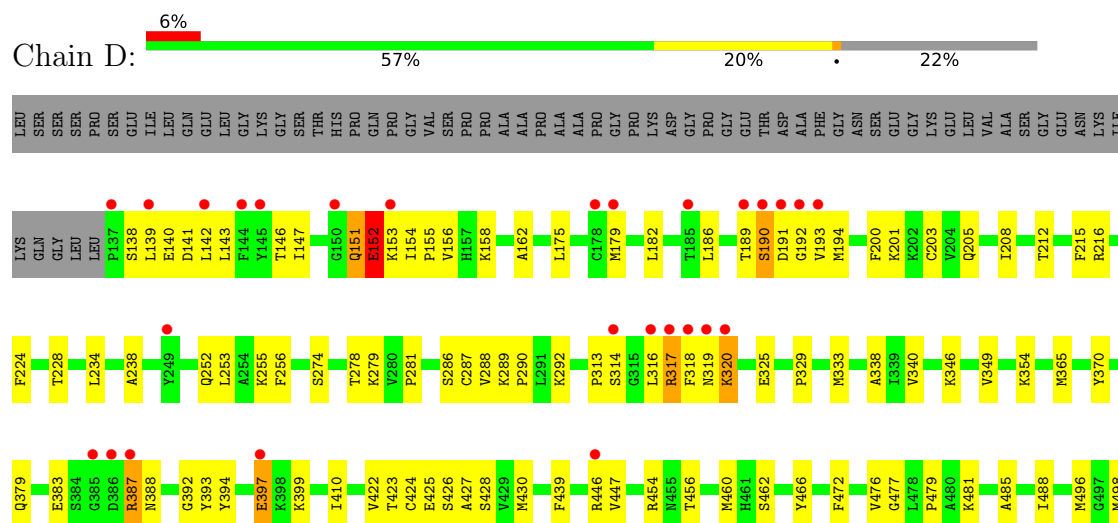
- Molecule 1: Glutaminase kidney isoform, mitochondrial

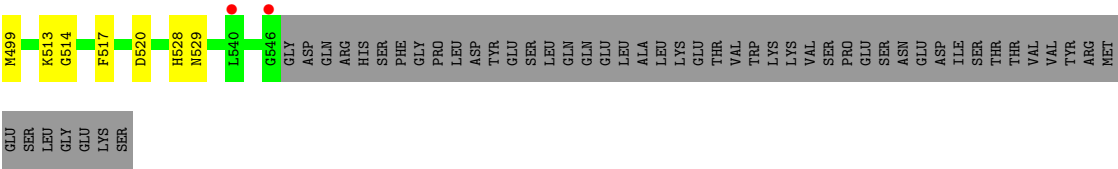


- Molecule 1: Glutaminase kidney isoform, mitochondrial



- Molecule 1: Glutaminase kidney isoform, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.98Å 138.82Å 176.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.10 – 2.75 48.10 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.10-2.75) 98.7 (48.10-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.229 , 0.293 0.232 , 0.291	Depositor DCC
R_{free} test set	2000 reflections (2.77%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	1.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12881	wwPDB-VP
Average B, all atoms (Å ²)	68.0	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 54.82 % 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 3.4551e-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: U27

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	1/3262 (0.0%)	0.92	22/4403 (0.5%)
1	B	0.63	6/3266 (0.2%)	1.01	26/4408 (0.6%)
1	C	0.53	2/3266 (0.1%)	0.83	12/4408 (0.3%)
1	D	0.48	2/3266 (0.1%)	0.82	12/4408 (0.3%)
All	All	0.54	11/13060 (0.1%)	0.90	72/17627 (0.4%)

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	C	0	1
1	D	0	1
All	All	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	280	VAL	CA-C	-13.32	1.39	1.52
1	B	312	GLU	CA-C	10.79	1.63	1.52
1	B	280	VAL	CA-C	-8.49	1.44	1.52
1	B	312	GLU	C-O	-6.77	1.17	1.24
1	C	190	SER	CA-C	6.75	1.62	1.52
1	D	387	ARG	CZ-NH2	-6.67	1.24	1.33
1	B	197	LYS	CG-CD	6.31	1.71	1.52
1	A	280	VAL	CA-C	5.97	1.57	1.53
1	B	397	GLU	N-CA	5.70	1.53	1.46
1	D	387	ARG	CZ-NH1	5.26	1.40	1.32
1	B	387	ARG	CZ-NH2	-5.06	1.26	1.33

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	312	GLU	O-C-N	12.78	131.52	121.55
1	C	317	ARG	CB-CG-CD	-10.25	87.73	111.30
1	A	202	LYS	CB-CG-CD	9.56	133.30	111.30
1	B	317	ARG	CG-CD-NE	-9.46	91.18	112.00
1	D	387	ARG	NE-CZ-NH1	9.17	130.67	121.50
1	B	216	ARG	CG-CD-NE	-8.94	92.33	112.00
1	C	217	ARG	CA-CB-CG	8.79	131.68	114.10
1	B	396	LYS	CA-CB-CG	8.23	130.56	114.10
1	B	540	LEU	CA-CB-CG	8.17	144.88	116.30
1	A	202	LYS	CG-CD-CE	-8.12	92.63	111.30
1	B	312	GLU	CA-C-N	-7.86	111.92	119.85
1	B	312	GLU	C-N-CA	-7.86	111.92	119.85
1	B	198	ASP	N-CA-CB	-7.81	99.07	110.47
1	C	217	ARG	CB-CG-CD	7.71	129.02	111.30
1	D	317	ARG	NE-CZ-NH1	-7.68	113.82	121.50
1	D	317	ARG	NH1-CZ-NH2	7.60	129.19	119.30
1	C	280	VAL	O-C-N	-7.33	112.74	121.10
1	B	198	ASP	CB-CA-C	7.30	122.01	109.24
1	B	540	LEU	CB-CA-C	-7.12	97.37	109.83
1	A	151	GLN	CA-C-N	-7.06	108.78	121.14
1	A	151	GLN	C-N-CA	-7.06	108.78	121.14
1	C	181	MET	CB-CG-SD	6.98	133.64	112.70
1	A	182	LEU	CA-CB-CG	6.96	140.66	116.30
1	B	177	GLU	CB-CA-C	6.59	122.82	110.63
1	A	255	LYS	CB-CG-CD	-6.53	96.28	111.30
1	B	538	LYS	CG-CD-CE	6.50	126.26	111.30
1	A	387	ARG	CB-CG-CD	6.45	126.12	111.30
1	B	317	ARG	CB-CA-C	-6.26	97.96	110.42
1	D	387	ARG	CD-NE-CZ	-6.22	115.69	124.40
1	B	205	GLN	CB-CG-CD	6.17	123.08	112.60
1	A	254	ALA	CA-C-N	6.16	128.81	120.38
1	A	254	ALA	C-N-CA	6.16	128.81	120.38
1	A	152	GLU	N-CA-CB	6.07	120.30	110.40
1	B	177	GLU	N-CA-CB	-6.00	100.98	110.22
1	B	540	LEU	CB-CG-CD1	-5.93	92.90	110.70
1	C	217	ARG	CB-CA-C	-5.89	103.19	111.80
1	A	359	MET	CA-CB-CG	-5.74	102.63	114.10
1	A	387	ARG	NE-CZ-NH1	-5.71	115.79	121.50
1	B	316	LEU	CA-C-N	5.65	132.33	121.54
1	B	316	LEU	C-N-CA	5.65	132.33	121.54
1	A	387	ARG	N-CA-CB	5.51	118.31	110.16
1	D	387	ARG	CA-CB-CG	-5.46	103.18	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	LYS	CB-CG-CD	-5.46	98.75	111.30
1	C	181	MET	CA-CB-CG	-5.45	103.19	114.10
1	A	387	ARG	CA-CB-CG	5.44	124.98	114.10
1	B	197	LYS	CA-C-N	5.43	131.82	122.09
1	B	197	LYS	C-N-CA	5.43	131.82	122.09
1	C	317	ARG	CD-NE-CZ	5.41	131.97	124.40
1	B	236	GLU	CA-CB-CG	-5.36	103.38	114.10
1	D	320	LYS	CB-CG-CD	5.36	123.63	111.30
1	B	153	LYS	CD-CE-NZ	5.35	129.02	111.90
1	A	152	GLU	CB-CG-CD	5.28	121.58	112.60
1	A	316	LEU	CA-C-N	-5.28	115.31	123.17
1	A	316	LEU	C-N-CA	-5.28	115.31	123.17
1	A	387	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	A	279	LYS	CG-CD-CE	5.27	123.41	111.30
1	B	317	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	B	397	GLU	CA-CB-CG	5.23	124.56	114.10
1	D	397	GLU	N-CA-CB	5.20	117.56	110.01
1	C	139	LEU	CB-CG-CD2	-5.20	95.10	110.70
1	C	212	THR	CA-CB-CG2	-5.19	101.67	110.50
1	D	387	ARG	NE-CZ-NH2	-5.19	114.53	119.20
1	B	317	ARG	CA-CB-CG	5.19	124.47	114.10
1	B	317	ARG	CD-NE-CZ	5.17	131.64	124.40
1	D	151	GLN	CA-C-N	5.08	131.25	121.54
1	D	151	GLN	C-N-CA	5.08	131.25	121.54
1	D	152	GLU	CA-C-N	5.05	130.65	122.53
1	D	152	GLU	C-N-CA	5.05	130.65	122.53
1	A	191	ASP	N-CA-CB	5.04	119.37	111.20
1	C	191	ASP	CA-C-N	5.03	131.26	121.41
1	C	191	ASP	C-N-CA	5.03	131.26	121.41
1	A	387	ARG	CG-CD-NE	-5.01	100.97	112.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	198	ASP	Sidechain
1	C	181	MET	Mainchain
1	D	190	SER	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	3190	0	3167	87	3
1	B	3194	0	3168	104	6
1	C	3194	0	3170	101	0
1	D	3194	0	3170	94	9
2	B	36	0	0	2	2
2	C	36	0	0	0	4
3	A	9	0	0	1	0
3	B	11	0	0	1	0
3	C	8	0	0	1	0
3	D	9	0	0	4	0
All	All	12881	0	12675	379	12

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 15.

All (379) 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:D:139:LEU:HD21	1:D:212:THR:HG21	1.40	1.00
1:A:288:VAL:HG13	1:A:292:LYS:HZ2	1.27	0.99
1:A:288:VAL:HG13	1:A:292:LYS:NZ	1.79	0.98
1:D:175:LEU:HB3	1:D:179:MET:HE1	1.53	0.90
1:A:279:LYS:HD3	1:A:425:GLU:HB2	1.56	0.85
1:B:314:SER:HB2	1:B:317:ARG:HH12	1.40	0.85
1:C:274:SER:HB3	1:C:278:THR:HG21	1.59	0.85
1:A:289:LYS:HA	1:A:292:LYS:HZ3	1.42	0.83
1:A:251:PRO:HB2	1:A:255:LYS:NZ	1.94	0.82
1:B:314:SER:HB2	1:B:317:ARG:NH1	1.93	0.82
1:B:315:GLY:C	1:B:317:ARG:H	1.87	0.82
1:C:143:LEU:HD12	1:C:212:THR:HG22	1.62	0.82
1:B:170:THR:HB	1:B:179:MET:HE2	1.62	0.81
1:A:202:LYS:O	1:A:202:LYS:HG2	1.81	0.80
1:C:189:THR:OG1	3:C:701:HOH:O	1.99	0.80
1:D:289:LYS:HD3	1:D:338:ALA:HB2	1.63	0.79
1:B:205:GLN:O	1:B:205:GLN:HG2	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ILE:HD11	1:B:253:LEU:HD13	1.65	0.78
1:D:314:SER:HB2	1:D:318:PHE:HB2	1.67	0.77
1:D:139:LEU:HD22	1:D:208:ILE:HG13	1.66	0.75
1:C:343:SER:HA	1:C:410:ILE:HD12	1.68	0.75
1:C:181:MET:HG3	1:C:181:MET:O	1.87	0.75
1:C:235:TYR:HD1	1:C:236:GLU:HG2	1.52	0.74
1:B:343:SER:HA	1:B:410:ILE:HD12	1.68	0.74
1:B:202:LYS:O	1:B:202:LYS:HG3	1.85	0.74
1:B:235:TYR:CD1	1:B:236:GLU:HG3	2.23	0.73
1:A:313:PRO:HG3	1:A:462:SER:HB2	1.70	0.72
1:D:286:SER:HG	1:D:466:TYR:HH	1.37	0.72
1:A:251:PRO:HB2	1:A:255:LYS:HZ3	1.55	0.71
1:D:427:ALA:HA	1:D:430:MET:HE3	1.71	0.71
1:A:279:LYS:HA	1:A:423:THR:HB	1.73	0.70
1:B:317:ARG:HG2	1:B:318:PHE:CD1	2.27	0.69
1:C:286:SER:OG	1:C:466:TYR:OH	2.11	0.69
1:D:274:SER:HB3	1:D:278:THR:HG21	1.72	0.69
1:A:147:ILE:O	1:A:158:LYS:NZ	2.25	0.69
1:C:155:PRO:HG3	1:C:194:MET:HE3	1.75	0.69
1:D:316:LEU:CD2	1:D:319:ASN:OD1	2.41	0.69
1:B:318:PHE:CD1	1:B:321:LEU:HD13	2.27	0.69
1:C:234:LEU:HD22	1:C:520:ASP:HB3	1.75	0.69
1:C:251:PRO:O	1:C:255:LYS:HD3	1.93	0.69
1:B:234:LEU:HD22	1:B:520:ASP:HB3	1.74	0.69
1:D:488:ILE:HD12	1:D:514:GLY:HA3	1.75	0.69
1:D:316:LEU:HD23	1:D:319:ASN:OD1	1.93	0.68
1:A:156:VAL:HG22	1:A:193:VAL:HG12	1.75	0.68
1:B:145:TYR:OH	1:B:197:LYS:HD2	1.93	0.68
1:A:152:GLU:HG3	1:A:153:LYS:HG3	1.74	0.68
1:C:422:VAL:HG11	1:C:430:MET:HE1	1.75	0.68
1:A:155:PRO:HG3	1:A:194:MET:HE2	1.75	0.67
1:C:143:LEU:HD22	1:C:200:PHE:HZ	1.60	0.67
1:C:316:LEU:HD21	1:C:467:ASP:HB3	1.76	0.67
1:A:530:TYR:CE1	1:D:479:PRO:HG3	2.30	0.67
1:D:175:LEU:O	1:D:179:MET:HE2	1.95	0.67
1:B:317:ARG:HG2	1:B:318:PHE:CE1	2.31	0.66
1:C:253:LEU:HD22	1:C:485:ALA:HA	1.76	0.65
1:B:498:MET:HE1	1:B:517:PHE:CE1	2.30	0.65
1:B:252:GLN:HB3	1:B:377:THR:HG22	1.78	0.65
1:C:422:VAL:CG1	1:C:430:MET:HE1	2.26	0.64
1:C:195:LEU:HA	1:C:199:LEU:HD23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:SER:HB2	1:C:318:PHE:HB2	1.78	0.64
1:B:260:LEU:HD23	1:B:501:TRP:CH2	2.32	0.63
1:A:265:VAL:HG22	1:A:498:MET:HE2	1.80	0.63
1:C:181:MET:SD	1:C:185:THR:HG23	2.38	0.63
1:C:252:GLN:HE21	1:C:376:ALA:C	2.07	0.63
1:B:285:GLN:HG3	1:B:484:VAL:HG12	1.79	0.63
1:C:208:ILE:O	1:C:212:THR:HG23	1.99	0.63
1:C:332:PRO:HB2	1:C:333:MET:HE2	1.79	0.63
1:B:302:THR:OG1	1:B:455:ASN:OD1	2.16	0.62
1:D:316:LEU:HD23	1:D:319:ASN:HD21	1.65	0.62
1:A:234:LEU:HD22	1:A:520:ASP:HB3	1.81	0.62
1:A:394:TYR:CZ	1:A:398:LYS:HE3	2.35	0.61
1:B:192:GLY:C	1:B:194:MET:H	2.07	0.61
1:B:153:LYS:HE2	1:B:196:ASP:CA	2.30	0.61
1:B:274:SER:HB3	1:B:278:THR:HG21	1.82	0.61
1:C:217:ARG:HG3	1:C:545:GLU:OE1	2.00	0.61
1:A:382:ARG:NH2	3:A:701:HOH:O	2.33	0.61
1:B:181:MET:O	1:B:185:THR:HG23	2.00	0.60
1:B:318:PHE:CE2	1:B:321:LEU:HD22	2.36	0.60
1:C:380:SER:HA	1:C:383:GLU:OE2	2.01	0.60
1:B:388:ASN:HB3	1:B:411:LEU:HD11	1.84	0.60
1:A:179:MET:HA	1:A:182:LEU:HD23	1.83	0.60
1:B:318:PHE:C	1:B:320:LYS:H	2.09	0.60
1:B:530:TYR:CE1	1:C:479:PRO:HG3	2.35	0.60
1:C:303:GLU:OE1	1:C:307:ARG:NH2	2.34	0.60
1:D:286:SER:OG	1:D:466:TYR:OH	2.10	0.60
1:B:496:MET:HE3	1:B:498:MET:SD	2.42	0.59
1:D:423:THR:N	1:D:426:SER:OG	2.30	0.59
1:C:198:ASP:HA	1:C:201:LYS:HB3	1.85	0.59
1:C:524:LEU:HD23	1:C:525:CYS:SG	2.43	0.59
1:D:139:LEU:CD2	1:D:212:THR:HG21	2.26	0.59
1:B:315:GLY:O	1:B:317:ARG:N	2.32	0.59
1:A:332:PRO:HD2	1:A:459:LEU:HD13	1.84	0.58
1:D:142:LEU:O	1:D:146:THR:HG23	2.03	0.58
1:C:484:VAL:HA	1:C:505:LEU:HD11	1.84	0.58
1:D:140:GLU:OE2	1:D:140:GLU:N	2.34	0.58
1:B:260:LEU:HD23	1:B:501:TRP:HH2	1.66	0.58
1:C:143:LEU:HD22	1:C:200:PHE:CZ	2.39	0.58
1:D:143:LEU:HD22	1:D:200:PHE:HZ	1.67	0.58
1:C:196:ASP:H	1:C:199:LEU:HB3	1.68	0.58
1:C:332:PRO:HD2	1:C:459:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:LEU:HD23	1:D:319:ASN:ND2	2.18	0.58
1:A:365:MET:HG3	1:A:447:VAL:HG11	1.86	0.58
1:C:169:ARG:HD2	1:C:272:ARG:HG3	1.86	0.58
1:C:316:LEU:HD11	1:C:467:ASP:CG	2.29	0.58
1:C:174:ARG:NH2	1:C:210:LEU:HD11	2.19	0.58
1:C:298:ASN:HD22	1:C:448:LEU:HA	1.69	0.58
1:B:318:PHE:CD2	1:B:321:LEU:HD22	2.39	0.58
1:A:249:TYR:CD1	1:A:250:ILE:HG23	2.39	0.57
1:B:318:PHE:HB3	1:B:321:LEU:HB2	1.85	0.57
1:D:139:LEU:O	1:D:139:LEU:HD23	2.03	0.57
1:A:289:LYS:HE3	1:A:338:ALA:CB	2.35	0.57
1:D:379:GLN:O	1:D:383:GLU:HG2	2.04	0.57
1:C:285:GLN:O	1:C:288:VAL:HG12	2.04	0.57
1:A:279:LYS:HD2	1:A:423:THR:OG1	2.04	0.57
1:B:209:VAL:O	1:B:213:GLN:HG3	2.05	0.57
1:C:138:SER:HB3	1:C:141:ASP:OD2	2.04	0.56
1:D:151:GLN:HB3	1:D:152:GLU:HG3	1.86	0.56
1:A:182:LEU:O	1:A:186:LEU:HB2	2.05	0.56
1:C:147:ILE:O	1:C:158:LYS:NZ	2.38	0.56
1:C:417:LEU:HD23	1:C:420:ILE:HD11	1.88	0.56
1:A:365:MET:HE2	1:A:448:LEU:HD11	1.88	0.56
1:B:176:LYS:O	1:B:180:ASP:N	2.35	0.56
1:A:346:LYS:HB3	1:A:354:LYS:HG2	1.88	0.56
1:C:443:THR:OG1	1:C:445:GLU:HG2	2.05	0.56
1:D:252:GLN:O	1:D:255:LYS:HG2	2.06	0.56
1:D:422:VAL:HG11	1:D:430:MET:HE1	1.87	0.56
1:D:189:THR:OG1	1:D:191:ASP:OD1	2.11	0.55
1:B:153:LYS:HE2	1:B:196:ASP:HA	1.88	0.55
1:B:224:PHE:O	1:B:228:THR:HG23	2.06	0.55
1:C:427:ALA:O	1:C:430:MET:HB2	2.06	0.55
1:C:498:MET:HE1	1:C:517:PHE:CE2	2.41	0.55
1:A:274:SER:HB3	1:A:278:THR:HG21	1.87	0.55
1:C:257:SER:HB3	1:C:260:LEU:HG	1.88	0.55
1:C:359:MET:HE1	1:C:420:ILE:HD13	1.89	0.55
1:B:235:TYR:CE2	1:B:261:TRP:CD1	2.95	0.55
1:B:529:ASN:ND2	1:C:529:ASN:OD1	2.38	0.55
1:C:314:SER:HB2	1:C:318:PHE:CB	2.37	0.55
1:C:298:ASN:ND2	1:C:448:LEU:HA	2.22	0.55
1:B:427:ALA:HB3	1:B:499:MET:HG2	1.89	0.54
1:B:332:PRO:HD2	1:B:459:LEU:HD13	1.89	0.54
1:D:325:GLU:HG3	3:D:707:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LEU:HB2	1:A:186:LEU:HD13	1.89	0.54
1:A:288:VAL:HG13	1:A:292:LYS:HZ1	1.67	0.54
1:D:216:ARG:HE	1:D:216:ARG:HA	1.71	0.54
1:D:154:ILE:HG22	1:D:155:PRO:O	2.07	0.54
1:A:182:LEU:O	1:A:186:LEU:HD13	2.08	0.54
1:D:175:LEU:O	1:D:179:MET:CE	2.56	0.54
1:A:250:ILE:HD12	1:A:252:GLN:HB2	1.90	0.53
1:C:492:VAL:HG21	1:C:496:MET:HE2	1.89	0.53
1:D:278:THR:O	1:D:425:GLU:HG3	2.08	0.53
1:A:148:ALA:O	1:A:149:GLU:HB2	2.08	0.53
1:D:143:LEU:HD12	1:D:212:THR:CG2	2.37	0.53
1:D:316:LEU:HD23	1:D:319:ASN:CG	2.33	0.53
1:D:439:PHE:CE2	1:D:446:ARG:HB2	2.44	0.53
1:A:153:LYS:HB3	1:A:194:MET:HG2	1.89	0.53
1:A:279:LYS:HZ2	1:A:426:SER:H	1.57	0.53
1:B:165:SER:HB2	1:B:225:MET:SD	2.49	0.53
1:C:224:PHE:O	1:C:228:THR:HG23	2.08	0.53
1:D:201:LYS:O	1:D:205:GLN:HB2	2.09	0.53
1:D:175:LEU:HB3	1:D:179:MET:CE	2.33	0.53
1:D:290:PRO:HA	1:D:333:MET:HE1	1.91	0.53
1:A:279:LYS:HD3	1:A:425:GLU:CB	2.34	0.52
1:B:317:ARG:NH1	1:B:318:PHE:HB2	2.24	0.52
1:A:289:LYS:HE3	1:A:338:ALA:HB2	1.90	0.52
2:B:601:U27:C01	1:C:317:ARG:HH22	2.22	0.52
1:D:290:PRO:HD3	1:D:481:LYS:HD3	1.91	0.52
1:B:319:ASN:N	3:B:701:HOH:O	2.41	0.52
1:C:488:ILE:HD12	1:C:514:GLY:HA3	1.92	0.51
1:B:288:VAL:O	1:B:292:LYS:HG2	2.10	0.51
1:B:379:GLN:OE1	1:B:382:ARG:HD3	2.11	0.51
1:C:365:MET:HG3	1:C:447:VAL:HG11	1.93	0.51
1:B:477:GLY:O	1:B:529:ASN:HB2	2.10	0.51
1:B:314:SER:CB	1:B:317:ARG:HH12	2.18	0.51
1:A:261:TRP:CE3	1:A:502:SER:HB2	2.46	0.51
1:B:289:LYS:HA	1:B:292:LYS:HE2	1.93	0.51
1:B:279:LYS:HD2	1:B:423:THR:HG21	1.92	0.51
1:A:157:HIS:O	1:A:161:THR:HG23	2.11	0.50
1:A:227:PHE:O	1:A:231:ILE:HG12	2.11	0.50
1:C:286:SER:HB3	1:C:289:LYS:NZ	2.26	0.50
1:A:250:ILE:CG2	1:A:380:SER:HB3	2.41	0.50
1:C:304:TYR:HA	1:C:307:ARG:HD2	1.93	0.50
2:B:601:U27:C01	1:C:317:ARG:NH2	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:THR:O	1:A:188:THR:HG22	2.12	0.50
1:B:278:THR:HG22	1:B:425:GLU:CG	2.42	0.50
1:B:524:LEU:HD23	1:B:525:CYS:SG	2.51	0.50
1:C:397:GLU:HG2	1:C:398:LYS:N	2.27	0.50
1:C:196:ASP:N	1:C:199:LEU:HB3	2.27	0.50
1:D:143:LEU:HD22	1:D:200:PHE:CZ	2.46	0.50
1:B:317:ARG:CZ	1:B:318:PHE:CD2	2.95	0.49
1:A:492:VAL:HG21	1:A:496:MET:HE2	1.93	0.49
1:B:278:THR:HG22	1:B:425:GLU:HG2	1.92	0.49
1:A:179:MET:HE2	1:A:182:LEU:HD21	1.94	0.49
1:A:317:ARG:HA	1:A:319:ASN:OD1	2.11	0.49
1:B:314:SER:C	1:B:317:ARG:NH1	2.70	0.49
1:A:432:ALA:HB1	1:A:441:PRO:HG2	1.95	0.49
1:D:224:PHE:O	1:D:228:THR:HG23	2.12	0.49
1:C:146:THR:HG21	1:C:216:ARG:HH21	1.77	0.49
1:C:162:ALA:HB1	1:C:215:PHE:HE1	1.78	0.49
1:C:318:PHE:C	1:C:320:LYS:H	2.20	0.49
1:D:143:LEU:HD12	1:D:212:THR:HG22	1.95	0.49
1:B:507:LYS:O	1:B:507:LYS:HG3	2.13	0.48
1:D:138:SER:OG	1:D:141:ASP:OD2	2.29	0.48
1:D:287:CYS:HA	1:D:481:LYS:HG2	1.95	0.48
1:D:316:LEU:CD2	1:D:319:ASN:HD21	2.25	0.48
1:C:288:VAL:O	1:C:292:LYS:HG2	2.13	0.48
1:D:365:MET:HG3	1:D:447:VAL:HG11	1.95	0.48
1:A:317:ARG:O	1:A:318:PHE:HD2	1.96	0.48
1:C:182:LEU:HD23	1:C:182:LEU:HA	1.75	0.48
1:B:264:SER:HB3	1:B:428:SER:HB3	1.96	0.48
1:C:204:VAL:HB	1:C:211:LEU:HD13	1.95	0.48
1:C:264:SER:OG	1:C:278:THR:CG2	2.62	0.48
1:B:192:GLY:C	1:B:194:MET:N	2.72	0.48
1:C:249:TYR:CE2	1:C:484:VAL:HG21	2.49	0.48
1:C:367:GLY:HA3	1:C:442:ILE:HD11	1.95	0.48
1:B:315:GLY:C	1:B:317:ARG:N	2.62	0.47
1:D:313:PRO:HG3	1:D:462:SER:HB2	1.95	0.47
1:A:265:VAL:HG22	1:A:498:MET:CE	2.43	0.47
1:A:477:GLY:O	1:A:529:ASN:HB2	2.14	0.47
1:B:365:MET:HG3	1:B:447:VAL:HG11	1.97	0.47
1:D:424:CYS:O	1:D:428:SER:HB3	2.14	0.47
1:B:374:SER:OG	1:B:377:THR:HG23	2.14	0.47
1:B:149:GLU:HB2	1:B:151:GLN:HB2	1.96	0.47
1:C:274:SER:CB	1:C:278:THR:HG21	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:PHE:O	1:A:148:ALA:N	2.48	0.47
1:D:456:THR:O	1:D:460:MET:HG3	2.15	0.47
1:B:317:ARG:HB3	1:B:318:PHE:H	1.59	0.47
1:C:278:THR:HG22	1:C:425:GLU:HG2	1.96	0.47
1:D:162:ALA:HB1	1:D:215:PHE:HE1	1.79	0.47
1:D:179:MET:HE2	1:D:179:MET:HB2	1.68	0.47
1:D:316:LEU:CD2	1:D:319:ASN:ND2	2.78	0.47
1:D:370:TYR:O	1:D:426:SER:HB2	2.14	0.47
1:A:362:LEU:HB3	1:A:430:MET:HE2	1.95	0.47
1:A:454:ARG:HD2	1:D:528:HIS:CG	2.50	0.47
1:D:255:LYS:HG3	1:D:256:PHE:N	2.29	0.47
1:A:322:PHE:O	1:A:323:LEU:HD23	2.15	0.47
1:C:359:MET:HE1	1:C:420:ILE:CD1	2.45	0.46
1:D:329:PRO:HG2	1:D:340:VAL:HG21	1.97	0.46
1:D:496:MET:HE3	1:D:498:MET:SD	2.55	0.46
1:B:527:PHE:CZ	1:B:542:PRO:HG2	2.49	0.46
1:D:279:LYS:HA	1:D:423:THR:HB	1.97	0.46
1:A:160:ILE:O	1:A:164:LYS:HG3	2.14	0.46
1:C:250:ILE:HB	1:C:380:SER:OG	2.15	0.46
1:D:234:LEU:HD22	1:D:520:ASP:HB3	1.96	0.46
1:A:289:LYS:HA	1:A:292:LYS:NZ	2.24	0.46
1:B:235:TYR:CE1	1:B:236:GLU:HG3	2.49	0.46
1:C:143:LEU:HD23	1:C:147:ILE:HD12	1.98	0.46
1:B:250:ILE:HB	1:B:380:SER:OG	2.16	0.46
1:A:144:PHE:O	1:A:148:ALA:HB2	2.16	0.46
1:C:379:GLN:O	1:C:383:GLU:OE1	2.33	0.46
1:D:238:ALA:O	1:D:513:LYS:HD3	2.16	0.46
1:B:249:TYR:CE1	1:B:484:VAL:HG21	2.51	0.46
1:D:477:GLY:O	1:D:529:ASN:HB2	2.15	0.46
1:C:148:ALA:O	1:C:151:GLN:HB2	2.16	0.46
1:A:154:ILE:HG22	1:A:155:PRO:O	2.15	0.46
1:A:251:PRO:HB2	1:A:255:LYS:HZ2	1.80	0.45
1:B:225:MET:HE3	1:B:225:MET:HB2	1.77	0.45
1:C:377:THR:HG22	1:C:419:SER:HB3	1.97	0.45
1:D:139:LEU:HD23	1:D:139:LEU:C	2.40	0.45
1:D:147:ILE:O	3:D:701:HOH:O	2.20	0.45
1:B:216:ARG:HB2	1:B:218:LYS:HG3	1.98	0.45
1:C:179:MET:HE3	1:C:179:MET:HB3	1.79	0.45
1:C:422:VAL:HG11	1:C:430:MET:CE	2.45	0.45
1:A:336:ALA:O	1:A:340:VAL:HG23	2.17	0.45
1:A:488:ILE:HD12	1:A:514:GLY:HA3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:THR:N	1:B:426:SER:OG	2.44	0.45
1:C:316:LEU:HD12	1:C:316:LEU:HA	1.61	0.45
1:A:143:LEU:HD13	1:A:212:THR:HG22	1.97	0.45
1:B:522:VAL:HG13	1:B:528:HIS:HB2	1.99	0.45
1:D:158:LYS:NZ	3:D:701:HOH:O	2.48	0.45
1:D:349:VAL:O	1:D:354:LYS:HE3	2.16	0.45
1:C:235:TYR:CD1	1:C:236:GLU:HG2	2.41	0.45
1:B:336:ALA:HA	1:B:391:ILE:HG21	1.98	0.45
1:B:387:ARG:O	1:B:391:ILE:HG13	2.16	0.45
1:C:427:ALA:HB3	1:C:499:MET:HG2	1.99	0.45
1:B:479:PRO:HD2	1:B:491:VAL:O	2.17	0.45
1:B:488:ILE:HD12	1:B:514:GLY:HA3	1.98	0.45
1:C:449:SER:O	1:C:453:VAL:HG23	2.17	0.45
1:A:178:CYS:O	1:A:182:LEU:HD23	2.16	0.45
1:A:281:PRO:HB3	1:A:370:TYR:HE2	1.81	0.45
1:D:316:LEU:CD2	1:D:319:ASN:CG	2.89	0.45
1:A:423:THR:N	1:A:426:SER:OG	2.44	0.44
1:D:346:LYS:O	1:D:354:LYS:HE2	2.16	0.44
1:B:252:GLN:CB	1:B:377:THR:HG22	2.45	0.44
1:B:281:PRO:HA	1:B:422:VAL:O	2.17	0.44
1:B:498:MET:HE1	1:B:517:PHE:HE1	1.77	0.44
1:A:192:GLY:C	1:A:194:MET:H	2.24	0.44
1:A:349:VAL:O	1:A:354:LYS:HE3	2.16	0.44
1:B:257:SER:HB3	1:B:260:LEU:HD13	2.00	0.44
1:B:527:PHE:HZ	1:B:542:PRO:HG2	1.82	0.44
1:A:387:ARG:O	1:A:391:ILE:HG13	2.17	0.44
1:D:153:LYS:HB2	1:D:194:MET:HE3	2.00	0.44
1:D:281:PRO:HA	1:D:422:VAL:O	2.17	0.44
1:A:423:THR:O	1:A:426:SER:OG	2.35	0.44
1:D:147:ILE:HG22	3:D:701:HOH:O	2.18	0.44
1:B:274:SER:CB	1:B:278:THR:HG21	2.48	0.44
1:C:197:LYS:O	1:C:201:LYS:HB2	2.18	0.44
1:C:235:TYR:CE2	1:C:261:TRP:CD1	3.05	0.43
1:C:281:PRO:HA	1:C:422:VAL:O	2.17	0.43
1:A:263:VAL:HG22	1:A:500:CYS:SG	2.59	0.43
1:A:454:ARG:HD2	1:D:528:HIS:CD2	2.53	0.43
1:B:148:ALA:HA	1:B:154:ILE:HG12	1.99	0.43
1:D:288:VAL:O	1:D:292:LYS:HG2	2.18	0.43
1:D:388:ASN:O	1:D:392:GLY:N	2.41	0.43
1:C:506:ASP:HB3	1:C:512:VAL:HG22	2.00	0.43
1:B:387:ARG:HA	1:B:390:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:SER:O	1:A:141:ASP:HB2	2.19	0.43
1:B:181:MET:HG2	1:B:202:LYS:O	2.19	0.43
1:C:467:ASP:HB2	1:C:508:MET:HE2	2.00	0.43
1:B:450:PRO:HG2	1:C:537:ALA:HB2	2.00	0.43
1:B:498:MET:HE2	1:B:498:MET:HB3	1.70	0.43
1:D:179:MET:HE2	1:D:179:MET:H	1.83	0.43
1:B:286:SER:HB3	1:B:289:LYS:HD2	2.01	0.43
1:C:219:PHE:HD2	1:C:271:GLN:HE21	1.67	0.43
1:C:427:ALA:HA	1:C:430:MET:HE3	2.00	0.43
1:A:358:VAL:HG11	1:A:417:LEU:CD2	2.49	0.42
1:D:182:LEU:O	1:D:186:LEU:HD12	2.19	0.42
1:C:252:GLN:NE2	1:C:376:ALA:O	2.51	0.42
1:A:250:ILE:HG21	1:A:380:SER:HB3	2.01	0.42
1:B:402:PRO:O	1:B:405:THR:OG1	2.26	0.42
1:C:267:THR:HA	1:C:496:MET:HA	2.01	0.42
1:D:253:LEU:HD22	1:D:485:ALA:HA	2.00	0.42
1:D:289:LYS:N	1:D:290:PRO:HD2	2.34	0.42
1:D:498:MET:HE1	1:D:517:PHE:CE1	2.54	0.42
1:C:154:ILE:HG22	1:C:155:PRO:O	2.19	0.42
1:C:477:GLY:O	1:C:529:ASN:HB2	2.19	0.42
1:D:397:GLU:C	1:D:399:LYS:H	2.27	0.42
1:D:498:MET:HE2	1:D:498:MET:HB3	1.86	0.42
1:B:391:ILE:HG22	1:B:395:LEU:HD11	2.01	0.42
1:B:252:GLN:OE1	1:B:252:GLN:N	2.51	0.42
1:B:317:ARG:HB3	1:B:317:ARG:HE	0.79	0.42
1:D:139:LEU:HD22	1:D:208:ILE:CG1	2.43	0.42
1:D:153:LYS:HB2	1:D:194:MET:HB3	2.01	0.42
1:B:153:LYS:HG2	1:B:196:ASP:HA	2.01	0.42
1:C:302:THR:OG1	1:C:455:ASN:ND2	2.46	0.42
1:A:279:LYS:NZ	1:A:426:SER:H	2.18	0.42
1:D:472:PHE:CZ	1:D:476:VAL:HG11	2.55	0.42
1:C:139:LEU:HA	1:C:139:LEU:HD23	1.66	0.42
1:C:225:MET:HE3	1:C:225:MET:HB3	1.88	0.42
1:C:318:PHE:C	1:C:320:LYS:N	2.77	0.42
1:D:318:PHE:C	1:D:320:LYS:H	2.28	0.42
1:A:148:ALA:O	1:A:149:GLU:CB	2.68	0.42
1:A:316:LEU:HD12	1:A:316:LEU:HA	1.74	0.42
1:B:318:PHE:C	1:B:320:LYS:N	2.73	0.42
1:C:422:VAL:HG12	1:C:430:MET:HE1	2.01	0.42
1:D:192:GLY:HA3	1:D:193:VAL:HA	1.72	0.42
1:A:318:PHE:C	1:A:320:LYS:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:GLY:HA2	1:B:500:CYS:O	2.20	0.41
1:B:162:ALA:HB1	1:B:215:PHE:HE1	1.84	0.41
1:B:267:THR:HA	1:B:496:MET:HA	2.01	0.41
1:B:313:PRO:HG3	1:B:462:SER:HB2	2.03	0.41
1:A:195:LEU:HG	1:A:200:PHE:HB2	2.02	0.41
1:A:289:LYS:N	1:A:290:PRO:HD2	2.35	0.41
1:B:154:ILE:HG22	1:B:155:PRO:O	2.20	0.41
1:D:179:MET:HE2	1:D:179:MET:N	2.36	0.41
1:B:167:GLY:HA3	1:B:224:PHE:CD2	2.56	0.41
1:D:316:LEU:HD21	1:D:319:ASN:OD1	2.17	0.41
1:D:289:LYS:HD3	1:D:338:ALA:CB	2.43	0.41
1:D:454:ARG:HH11	1:D:454:ARG:HD3	1.73	0.41
1:A:156:VAL:HG21	1:A:186:LEU:HD21	2.03	0.41
1:B:270:GLY:O	1:B:272:ARG:HG2	2.21	0.41
1:D:156:VAL:HG13	1:D:193:VAL:O	2.21	0.41
1:A:195:LEU:HD12	1:A:199:LEU:HG	2.03	0.41
1:A:411:LEU:HD13	1:A:411:LEU:HA	1.78	0.41
1:B:250:ILE:HG13	1:B:253:LEU:H	1.86	0.41
1:B:332:PRO:CD	1:B:459:LEU:HD13	2.51	0.41
1:D:410:ILE:HD13	1:D:410:ILE:HA	1.89	0.41
1:A:182:LEU:O	1:A:186:LEU:CD1	2.68	0.41
1:A:225:MET:HE2	1:A:225:MET:HA	2.03	0.41
1:A:498:MET:HE2	1:A:498:MET:HB3	1.77	0.41
1:C:456:THR:O	1:C:460:MET:HG3	2.21	0.40
1:D:427:ALA:HB3	1:D:499:MET:HG2	2.04	0.40
1:A:412:ASP:O	1:A:416:GLN:HG2	2.21	0.40
1:B:484:VAL:HA	1:B:505:LEU:HD11	2.03	0.40
1:C:286:SER:HB3	1:C:289:LYS:HZ2	1.85	0.40
1:B:529:ASN:HD21	1:C:529:ASN:CG	2.27	0.40
1:C:153:LYS:HB3	1:C:195:LEU:O	2.21	0.40
1:D:182:LEU:HD23	1:D:203:CYS:SG	2.61	0.40
1:A:250:ILE:HD11	1:A:253:LEU:HG	2.03	0.40
1:B:364:LYS:HE2	1:B:445:GLU:OE1	2.21	0.40
1:D:143:LEU:HD12	1:D:212:THR:HG23	2.03	0.40

All (12) 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:317:ARG:NH1	2:C:601:U27:C32[4_445]	1.41	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:LYS:NZ	2:B:601:U27:C36[4_445]	1.43	0.77
1:A:317:ARG:NH1	2:C:601:U27:C33[4_445]	1.44	0.76
1:D:317:ARG:NH1	2:C:601:U27:C25[4_445]	1.45	0.75
1:D:320:LYS:NZ	2:B:601:U27:C35[4_445]	1.47	0.73
1:B:387:ARG:NH2	1:D:394:TYR:O[4_545]	1.79	0.41
1:A:242:SER:OG	1:B:303:GLU:OE1[1_455]	1.82	0.38
1:B:394:TYR:O	1:D:387:ARG:NH2[4_545]	1.95	0.25
1:B:397:GLU:OE2	1:D:387:ARG:NE[4_545]	1.98	0.22
1:B:393:TYR:O	1:D:387:ARG:NH1[4_545]	2.04	0.16
1:B:387:ARG:NH1	1:D:393:TYR:O[4_545]	2.10	0.10
1:D:317:ARG:NH1	2:C:601:U27:C26[4_445]	2.16	0.04

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%)	389 (96%)	18 (4%)	0	100	100
1	B	408/527 (77%)	385 (94%)	22 (5%)	1 (0%)	43	64
1	C	408/527 (77%)	388 (95%)	19 (5%)	1 (0%)	43	64
1	D	408/527 (77%)	385 (94%)	21 (5%)	2 (0%)	24	43
All	All	1631/2108 (77%)	1547 (95%)	80 (5%)	4 (0%)	43	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	192	GLY
1	D	152	GLU
1	D	190	SER
1	B	316	LEU

5.3.2 Protein sidechains [i](#)

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 (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	273	HIS
1	B	319	ASN
1	B	335	ASN
1	B	388	ASN
1	B	471	GLN
1	B	516	HIS
1	C	298	ASN
1	C	347	GLN
1	C	368	ASN
1	C	388	ASN
1	C	471	GLN
1	D	187	GLN
1	D	241	GLN
1	D	347	GLN
1	D	368	ASN
1	D	416	GLN
1	D	455	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	U27	C	601	-	40,40,40	4.02	24 (60%)	50,54,54	5.94	30 (60%)
2	U27	B	601	-	40,40,40	4.03	32 (80%)	50,54,54	6.09	29 (58%)

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	U27	C	601	-	-	10/22/33/33	0/5/5/5
2	U27	B	601	-	-	8/22/33/33	0/5/5/5

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	U27	C04-S29	10.73	1.91	1.73
2	B	601	U27	C17-S28	9.14	1.89	1.73
2	C	601	U27	C25-C24	9.07	1.58	1.38
2	B	601	U27	C04-S29	8.74	1.88	1.73
2	C	601	U27	C14-S28	8.19	1.89	1.75
2	B	601	U27	C20-C21	7.75	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	U27	C14-S28	7.21	1.88	1.75
2	B	601	U27	C02-N03	7.03	1.50	1.37
2	C	601	U27	C17-S28	6.80	1.85	1.73
2	C	601	U27	C02-N03	6.09	1.48	1.37
2	C	601	U27	C19-N18	5.67	1.47	1.37
2	C	601	U27	C25-C26	5.64	1.48	1.38
2	C	601	U27	C23-C24	5.64	1.50	1.38
2	B	601	U27	C04-N03	5.49	1.46	1.38
2	B	601	U27	C01-C31	5.44	1.60	1.51
2	B	601	U27	C19-N18	5.33	1.47	1.37
2	C	601	U27	C07-S29	5.13	1.86	1.75
2	B	601	U27	C12-N08	5.09	1.56	1.46
2	C	601	U27	C26-C21	4.70	1.48	1.38
2	B	601	U27	C17-N18	4.25	1.44	1.38
2	C	601	U27	C01-C02	4.20	1.60	1.52
2	C	601	U27	C22-C21	4.04	1.46	1.38
2	B	601	U27	C01-C02	3.94	1.60	1.52
2	B	601	U27	C07-N06	3.82	1.38	1.31
2	B	601	U27	C07-N08	3.80	1.43	1.34
2	C	601	U27	C17-N16	3.76	1.36	1.31
2	C	601	U27	C01-C31	3.71	1.57	1.51
2	B	601	U27	C36-C31	3.58	1.46	1.38
2	B	601	U27	C17-N16	3.45	1.36	1.31
2	B	601	U27	C04-N05	3.11	1.35	1.31
2	B	601	U27	C07-S29	3.09	1.82	1.75
2	B	601	U27	C12-C11	3.07	1.57	1.52
2	C	601	U27	C04-N03	3.04	1.42	1.38
2	B	601	U27	C22-C21	3.02	1.44	1.38
2	C	601	U27	C12-N08	2.98	1.52	1.46
2	B	601	U27	C20-C19	2.90	1.58	1.52
2	C	601	U27	C20-C21	-2.88	1.47	1.51
2	C	601	U27	C35-C34	2.77	1.44	1.38
2	B	601	U27	N16-N15	-2.66	1.34	1.39
2	C	601	U27	C34-C33	2.61	1.44	1.38
2	B	601	U27	C35-C34	2.60	1.44	1.38
2	C	601	U27	C23-C22	-2.55	1.34	1.38
2	B	601	U27	C26-C21	2.49	1.43	1.38
2	B	601	U27	C35-C36	2.49	1.43	1.38
2	C	601	U27	C35-C36	2.47	1.43	1.38
2	C	601	U27	N06-N05	-2.35	1.34	1.39
2	B	601	U27	C23-C24	2.34	1.43	1.38
2	B	601	U27	C23-C22	2.32	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	U27	C36-C31	2.28	1.43	1.38
2	B	601	U27	C25-C26	2.26	1.42	1.38
2	B	601	U27	C32-C31	2.25	1.43	1.38
2	B	601	U27	C14-N15	2.25	1.31	1.29
2	B	601	U27	C25-C24	2.17	1.43	1.38
2	C	601	U27	C12-C11	2.16	1.56	1.52
2	B	601	U27	C34-C33	2.16	1.43	1.38
2	B	601	U27	C10-C09	2.04	1.56	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	U27	C20-C19-N18	18.31	136.73	114.40
2	B	601	U27	N03-C04-N05	18.13	137.00	120.81
2	B	601	U27	C20-C19-N18	13.89	131.34	114.40
2	B	601	U27	C14-N15-N16	12.35	120.07	105.84
2	B	601	U27	S29-C04-N05	-11.99	101.14	114.52
2	C	601	U27	C14-N15-N16	11.97	119.62	105.84
2	C	601	U27	S29-C04-N05	-11.90	101.23	114.52
2	B	601	U27	S28-C17-N16	-11.22	101.99	114.52
2	C	601	U27	C11-O13-C14	11.13	125.03	117.71
2	C	601	U27	S28-C17-N16	-10.88	102.37	114.52
2	B	601	U27	N08-C07-N06	10.40	137.01	116.91
2	C	601	U27	N03-C04-N05	10.31	130.02	120.81
2	C	601	U27	C09-N08-C12	-9.89	100.83	112.38
2	C	601	U27	S28-C14-N15	-9.85	104.20	117.59
2	B	601	U27	S28-C14-N15	-9.54	104.62	117.59
2	B	601	U27	C09-N08-C12	-9.45	101.34	112.38
2	B	601	U27	C11-O13-C14	9.06	123.67	117.71
2	B	601	U27	C01-C02-N03	8.75	125.08	114.40
2	B	601	U27	N18-C17-N16	8.37	128.29	120.81
2	C	601	U27	N08-C07-N06	7.99	132.35	116.91
2	C	601	U27	C04-N05-N06	7.83	121.99	112.02
2	B	601	U27	C17-N16-N15	7.45	121.50	112.02
2	B	601	U27	S29-C07-N06	-7.28	101.84	114.44
2	C	601	U27	O27-C19-C20	-7.27	106.24	121.99
2	C	601	U27	C17-N16-N15	7.24	121.23	112.02
2	C	601	U27	C07-N06-N05	7.05	120.98	107.08
2	B	601	U27	C19-N18-C17	6.78	135.27	123.69
2	C	601	U27	S29-C07-N06	-6.77	102.73	114.44
2	B	601	U27	C07-N06-N05	6.75	120.39	107.08
2	B	601	U27	C04-N05-N06	6.27	120.00	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	U27	N18-C17-N16	6.04	126.20	120.81
2	C	601	U27	C01-C02-N03	6.03	121.75	114.40
2	C	601	U27	S28-C17-N18	5.75	131.42	123.72
2	B	601	U27	O27-C19-N18	-5.39	112.23	122.44
2	C	601	U27	C24-C25-C26	-4.58	114.59	120.24
2	B	601	U27	S28-C17-N18	4.43	129.66	123.72
2	B	601	U27	C10-C09-N08	4.04	108.13	102.93
2	C	601	U27	C12-N08-C07	3.84	130.55	123.83
2	C	601	U27	S29-C04-N03	3.75	128.75	123.72
2	C	601	U27	O13-C14-S28	3.57	123.83	116.13
2	B	601	U27	C21-C20-C19	3.53	122.87	112.33
2	B	601	U27	C12-N08-C07	3.46	129.88	123.83
2	C	601	U27	S29-C07-N08	3.44	124.91	120.31
2	C	601	U27	C23-C22-C21	3.40	125.39	120.61
2	B	601	U27	O13-C11-C12	3.09	115.56	108.30
2	C	601	U27	C02-N03-C04	2.93	128.69	123.69
2	C	601	U27	C09-N08-C07	-2.92	118.72	123.83
2	C	601	U27	O27-C19-N18	-2.87	117.00	122.44
2	C	601	U27	C17-S28-C14	2.87	92.56	86.65
2	B	601	U27	O13-C14-S28	2.83	122.25	116.13
2	C	601	U27	O13-C11-C12	2.72	114.69	108.30
2	C	601	U27	C10-C09-N08	2.66	106.35	102.93
2	B	601	U27	O27-C19-C20	-2.60	116.36	121.99
2	B	601	U27	O30-C02-C01	-2.54	116.48	121.99
2	B	601	U27	C17-S28-C14	2.51	91.82	86.65
2	B	601	U27	O30-C02-N03	-2.11	118.44	122.44
2	B	601	U27	C09-N08-C07	-2.10	120.17	123.83
2	B	601	U27	O13-C11-C10	2.04	119.74	106.48
2	C	601	U27	C31-C01-C02	2.00	118.30	112.33

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	U27	N05-C04-N03-C02
2	B	601	U27	S29-C04-N03-C02
2	B	601	U27	N06-C07-N08-C09
2	B	601	U27	S29-C07-N08-C09
2	B	601	U27	S29-C07-N08-C12
2	B	601	U27	C10-C11-O13-C14
2	C	601	U27	N16-C17-N18-C19
2	C	601	U27	S28-C17-N18-C19

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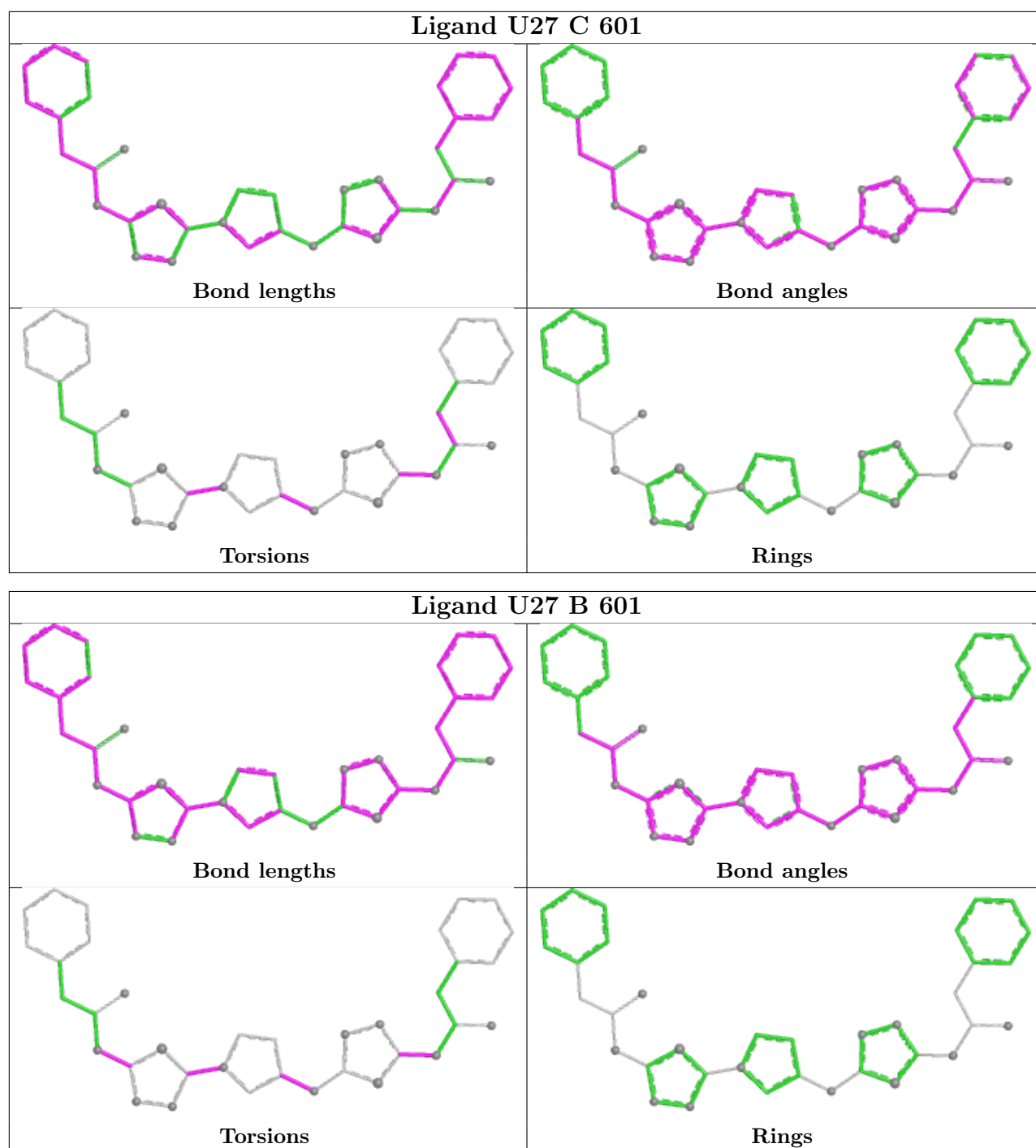
Mol	Chain	Res	Type	Atoms
2	C	601	U27	N06-C07-N08-C12
2	C	601	U27	S29-C07-N08-C12
2	C	601	U27	C12-C11-O13-C14
2	B	601	U27	N06-C07-N08-C12
2	C	601	U27	N06-C07-N08-C09
2	C	601	U27	S29-C07-N08-C09
2	B	601	U27	S28-C17-N18-C19
2	C	601	U27	C10-C11-O13-C14
2	C	601	U27	N18-C19-C20-C21
2	C	601	U27	O27-C19-C20-C21

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	U27	0	4
2	B	601	U27	2	2

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%)	0.49	35 (8%)	16 16	44, 61, 116, 204	0
1	B	410/527 (77%)	0.58	40 (9%)	13 12	41, 59, 124, 218	0
1	C	410/527 (77%)	0.61	35 (8%)	16 17	41, 61, 114, 176	0
1	D	410/527 (77%)	0.43	29 (7%)	22 22	41, 58, 105, 188	0
All	All	1639/2108 (77%)	0.53	139 (8%)	16 17	41, 60, 116, 218	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	249	TYR	6.0
1	D	318	PHE	5.9
1	C	316	LEU	5.5
1	D	249	TYR	5.5
1	B	318	PHE	5.3
1	A	189	THR	5.3
1	B	189	THR	5.0
1	C	253	LEU	4.9
1	B	193	VAL	4.7
1	B	253	LEU	4.7
1	A	198	ASP	4.6
1	C	181	MET	4.5
1	A	243	GLY	4.4
1	B	546	GLY	4.4
1	A	193	VAL	4.3
1	C	318	PHE	4.2
1	C	169	ARG	4.2
1	B	397	GLU	4.1
1	C	192	GLY	4.0
1	D	190	SER	4.0
1	B	316	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	190	SER	4.0
1	C	387	ARG	4.0
1	B	387	ARG	3.9
1	D	193	VAL	3.9
1	B	249	TYR	3.9
1	C	145	TYR	3.8
1	C	301	GLY	3.8
1	C	191	ASP	3.8
1	C	150	GLY	3.7
1	A	137	PRO	3.7
1	D	145	TYR	3.6
1	B	188	THR	3.6
1	B	137	PRO	3.6
1	B	256	PHE	3.5
1	B	317	ARG	3.5
1	C	319	ASN	3.4
1	D	546	GLY	3.4
1	D	387	ARG	3.4
1	B	319	ASN	3.4
1	D	189	THR	3.3
1	A	279	LYS	3.3
1	B	153	LYS	3.3
1	A	188	THR	3.3
1	A	145	TYR	3.3
1	B	139	LEU	3.2
1	C	188	THR	3.2
1	B	258	PRO	3.2
1	A	318	PHE	3.2
1	C	186	LEU	3.2
1	C	189	THR	3.2
1	A	190	SER	3.1
1	C	194	MET	3.1
1	B	540	LEU	3.0
1	D	397	GLU	3.0
1	C	202	LYS	3.0
1	A	156	VAL	3.0
1	A	213	GLN	3.0
1	C	187	GLN	3.0
1	A	202	LYS	3.0
1	A	317	ARG	3.0
1	D	540	LEU	2.9
1	C	137	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	199	LEU	2.9
1	B	250	ILE	2.9
1	A	319	ASN	2.8
1	B	145	TYR	2.8
1	A	191	ASP	2.8
1	D	191	ASP	2.8
1	A	194	MET	2.8
1	A	186	LEU	2.8
1	C	317	ARG	2.8
1	B	396	LYS	2.7
1	D	139	LEU	2.7
1	C	203	CYS	2.7
1	D	144	PHE	2.7
1	A	540	LEU	2.7
1	D	142	LEU	2.7
1	C	193	VAL	2.6
1	B	251	PRO	2.6
1	D	137	PRO	2.6
1	C	139	LEU	2.6
1	B	202	LYS	2.6
1	A	192	GLY	2.6
1	C	302	THR	2.6
1	B	167	GLY	2.6
1	A	150	GLY	2.5
1	B	205	GLN	2.5
1	A	248	ASP	2.5
1	C	383	GLU	2.5
1	B	148	ALA	2.5
1	A	397	GLU	2.5
1	A	251	PRO	2.5
1	A	240	LYS	2.5
1	C	255	LYS	2.4
1	A	153	LYS	2.4
1	D	185	THR	2.4
1	C	198	ASP	2.4
1	C	546	GLY	2.4
1	B	255	LYS	2.4
1	A	220	VAL	2.4
1	B	149	GLU	2.4
1	B	225	MET	2.4
1	B	466	TYR	2.3
1	A	387	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	320	LYS	2.3
1	C	283	CYS	2.2
1	B	213	GLN	2.2
1	B	156	VAL	2.2
1	B	186	LEU	2.2
1	D	153	LYS	2.2
1	B	181	MET	2.2
1	C	157	HIS	2.2
1	B	194	MET	2.2
1	D	150	GLY	2.1
1	B	248	ASP	2.1
1	A	200	PHE	2.1
1	C	256	PHE	2.1
1	A	545	GLU	2.1
1	D	317	ARG	2.1
1	A	351	ASN	2.1
1	D	319	ASN	2.1
1	B	192	GLY	2.1
1	D	192	GLY	2.1
1	B	198	ASP	2.1
1	C	163	LEU	2.1
1	B	243	GLY	2.1
1	D	386	ASP	2.1
1	A	152	GLU	2.1
1	D	179	MET	2.1
1	D	178	CYS	2.1
1	D	385	GLY	2.1
1	D	446	ARG	2.0
1	A	185	THR	2.0
1	B	379	GLN	2.0
1	D	316	LEU	2.0
1	C	525	CYS	2.0
1	A	544	ARG	2.0
1	D	314	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

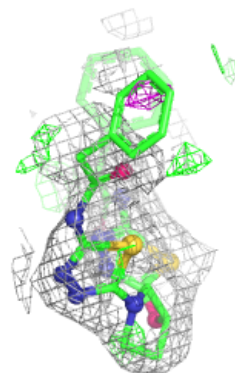
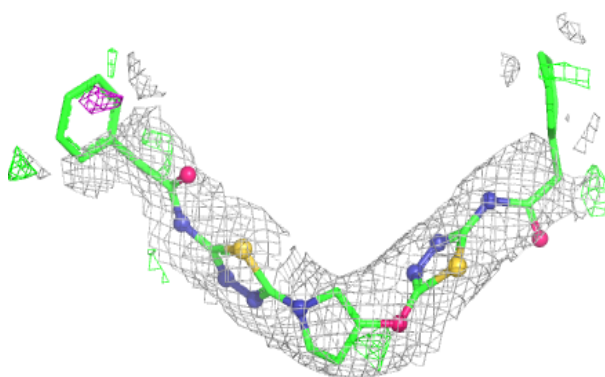
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	U27	C	601	36/36	0.83	0.19	56,103,168,176	0
2	U27	B	601	36/36	0.87	0.20	67,93,138,140	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.

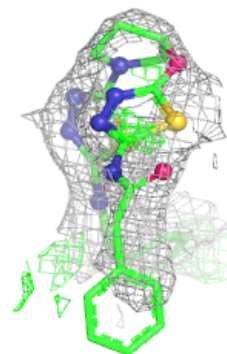
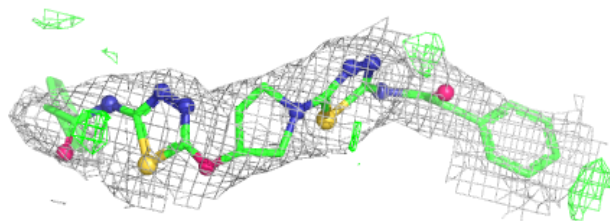
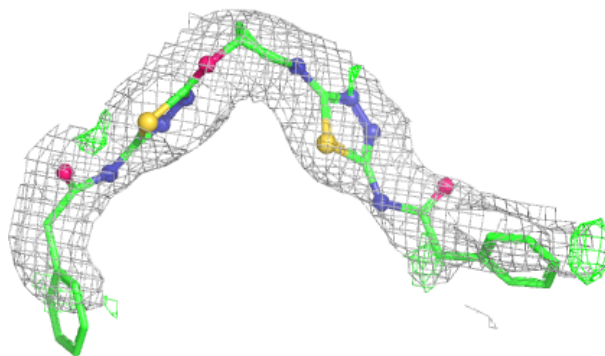
Electron density around U27 C 601:

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 U27 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.