



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2020 – 11:12 AM EDT

PDB ID : 6UMC
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

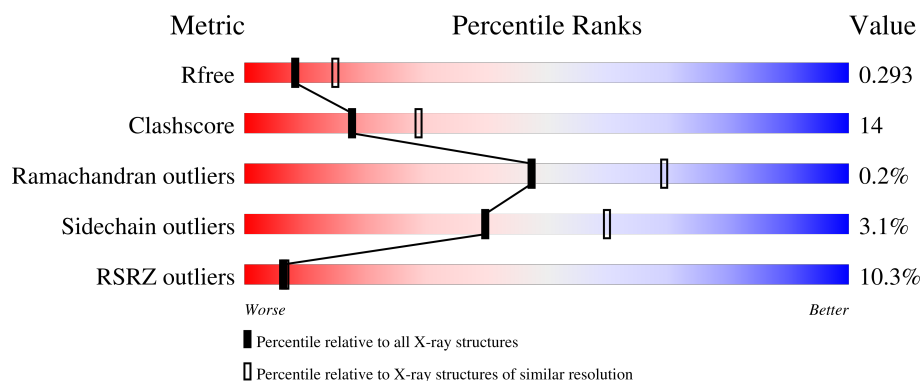
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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

Mol	Chain	Length	Quality of chain
1	A	527	<div> <div>9%</div> <div>57%</div> <div>19%</div> <div>•</div> <div>22%</div> </div>
1	B	527	<div> <div>9%</div> <div>52%</div> <div>23%</div> <div>•</div> <div>22%</div> </div>
1	C	527	<div> <div>8%</div> <div>54%</div> <div>21%</div> <div>•</div> <div>22%</div> </div>
1	D	527	<div> <div>6%</div> <div>56%</div> <div>20%</div> <div>•</div> <div>22%</div> </div>

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.

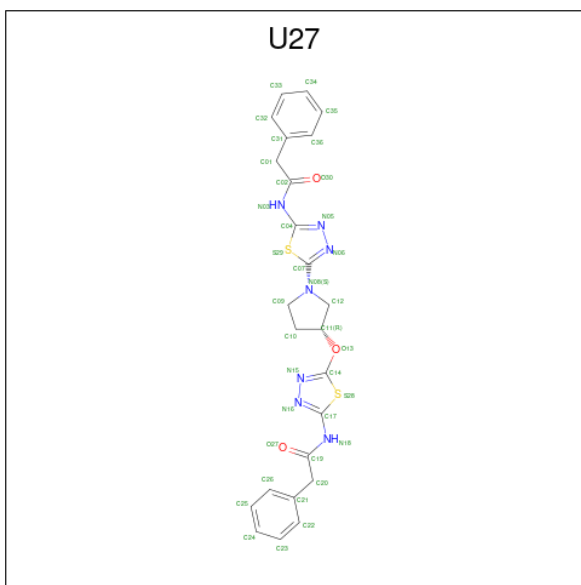
- Molecule 1 is a protein called Glutaminase kidney isoform, mitochondrial.

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

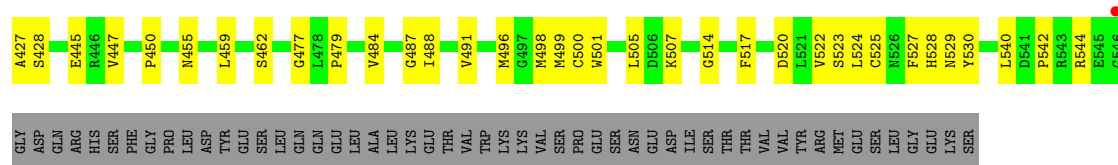
- Molecule 2 is 2-phenyl-N-{5-[(3R)-3-({5-[(phenylacetyl)amino]-1,3,4-thiadiazol-2-yl}oxy)pyrrolidin-1-yl]-1,3,4-thiadiazol-2-yl}acetamide (three-letter code: U27) (formula: C₂₄H₂₃N₇O₃S₂) (labeled as "Ligand of Interest" by author).



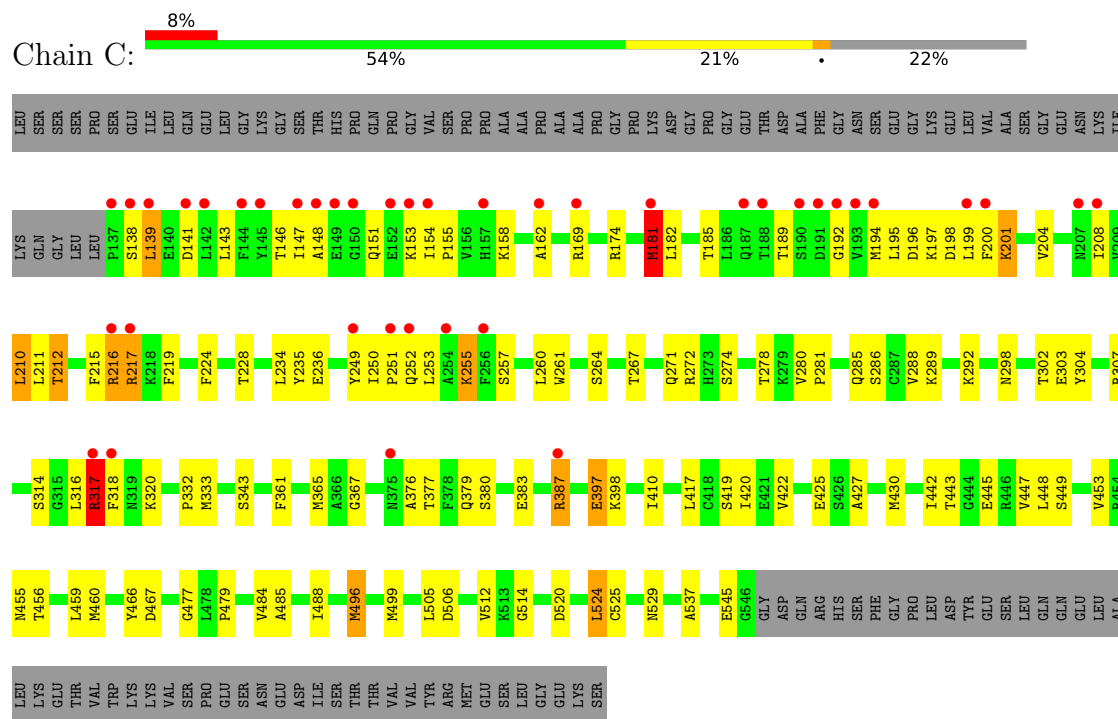
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 36	C 24	N 7	O 3	S 2	0	0
2	D	1	Total 36	C 24	N 7	O 3	S 2	0	0

- Molecule 3 is water.

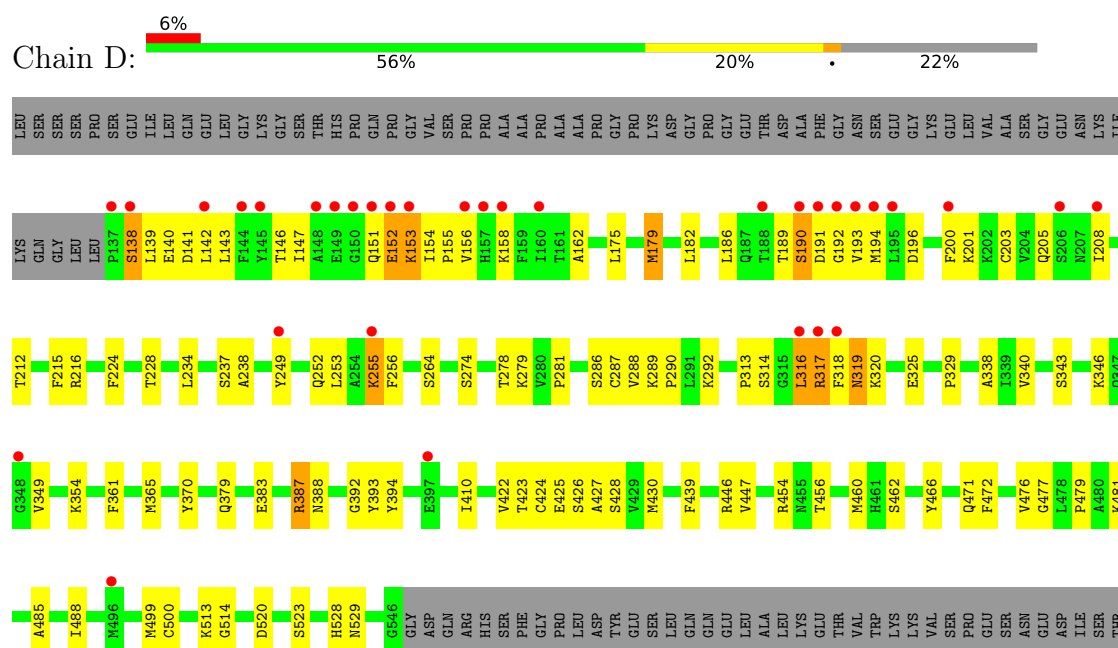
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	9	Total O 9 9	0	0
3	B	11	Total O 11 11	0	0
3	C	8	Total O 8 8	0	0
3	D	9	Total O 9 9	0	0



- Molecule 1: Glutaminase kidney isoform, mitochondrial



- Molecule 1: Glutaminase kidney isoform, mitochondrial



THR
VAL
VAL
TYR
ARG
MET
GLU
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	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 0.229 , 0.293	Depositor DCC
R_{free} test set	1780 reflections (2.79%)	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)	0.30 , 22.1	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	0.94	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 [i](#)

5.1 Standard geometry [i](#)

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	0.53	2/3262 (0.1%)	0.87	15/4403 (0.3%)
1	B	0.63	2/3266 (0.1%)	1.00	25/4408 (0.6%)
1	C	0.55	3/3266 (0.1%)	0.84	12/4408 (0.3%)
1	D	0.55	4/3266 (0.1%)	0.87	9/4408 (0.2%)
All	All	0.57	11/13060 (0.1%)	0.89	61/17627 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	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	B	397	GLU	CD-OE2	-7.16	1.17	1.25
1	D	387	ARG	CZ-NH2	-6.37	1.24	1.33
1	C	397	GLU	CD-OE2	-6.33	1.18	1.25
1	A	397	GLU	CG-CD	-5.61	1.43	1.51
1	B	197	LYS	CG-CD	5.57	1.71	1.52
1	D	387	ARG	CZ-NH1	5.43	1.40	1.33
1	C	280	VAL	CA-C	-5.40	1.39	1.52
1	A	202	LYS	CD-CE	5.40	1.64	1.51
1	D	500	CYS	CB-SG	-5.30	1.73	1.81
1	D	317	ARG	CB-CG	-5.28	1.38	1.52
1	C	387	ARG	CG-CD	5.14	1.64	1.51

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	387	ARG	NE-CZ-NH1	20.74	130.67	120.30
1	D	317	ARG	NE-CZ-NH1	-12.97	113.82	120.30
1	B	540	LEU	CA-CB-CG	12.86	144.88	115.30
1	B	387	ARG	NE-CZ-NH1	11.90	126.25	120.30
1	D	387	ARG	NE-CZ-NH2	-11.54	114.53	120.30
1	A	182	LEU	CA-CB-CG	11.03	140.66	115.30
1	B	540	LEU	CB-CG-CD1	-10.65	92.90	111.00
1	C	317	ARG	NE-CZ-NH2	-10.51	115.04	120.30
1	B	216	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	B	216	ARG	NE-CZ-NH1	10.09	125.35	120.30
1	B	317	ARG	CG-CD-NE	-9.82	91.18	111.80
1	B	387	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	C	139	LEU	CB-CG-CD2	-9.35	95.10	111.00
1	B	216	ARG	CG-CD-NE	-9.27	92.33	111.80
1	C	317	ARG	CB-CG-CD	-9.18	87.73	111.60
1	B	198	ASP	CB-CG-OD1	-9.03	110.17	118.30
1	A	387	ARG	NE-CZ-NH1	-9.01	115.79	120.30
1	D	317	ARG	NH1-CZ-NH2	8.90	129.19	119.40
1	D	316	LEU	CB-CG-CD2	-8.70	96.21	111.00
1	A	139	LEU	CB-CG-CD2	-8.58	96.42	111.00
1	A	202	LYS	CB-CG-CD	8.35	133.30	111.60
1	C	217	ARG	CA-CB-CG	8.31	131.68	113.40
1	B	317	ARG	NE-CZ-NH1	-8.10	116.25	120.30
1	B	396	LYS	CA-CB-CG	7.80	130.56	113.40
1	C	212	THR	CA-CB-CG2	-7.66	101.67	112.40
1	B	153	LYS	CD-CE-NZ	7.53	129.02	111.70
1	A	387	ARG	NE-CZ-NH2	7.29	123.94	120.30
1	D	317	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	C	181	MET	CB-CG-SD	7.08	133.64	112.40
1	B	540	LEU	CB-CG-CD2	7.01	122.92	111.00
1	B	540	LEU	CB-CA-C	-6.75	97.37	110.20
1	C	217	ARG	CB-CG-CD	6.70	129.02	111.60
1	D	316	LEU	CA-CB-CG	-6.62	100.07	115.30
1	A	202	LYS	CG-CD-CE	-6.42	92.63	111.90
1	B	198	ASP	N-CA-CB	-6.40	99.07	110.60
1	A	359	MET	CA-CB-CG	-6.28	102.63	113.30
1	A	198	ASP	CB-CG-OD1	6.24	123.92	118.30
1	B	317	ARG	CB-CA-C	-6.21	97.97	110.40
1	B	177	GLU	CB-CA-C	6.21	122.82	110.40
1	D	320	LYS	CD-CE-NZ	6.07	125.65	111.70
1	C	317	ARG	CD-NE-CZ	5.98	131.97	123.60
1	C	317	ARG	NE-CZ-NH1	5.97	123.28	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	181	MET	CA-CB-CG	-5.95	103.19	113.30
1	A	255	LYS	CB-CG-CD	-5.89	96.28	111.60
1	C	181	MET	CG-SD-CE	5.84	109.55	100.20
1	B	198	ASP	CB-CA-C	5.80	122.01	110.40
1	A	186	LEU	CA-CB-CG	-5.80	101.97	115.30
1	B	317	ARG	CD-NE-CZ	5.74	131.64	123.60
1	D	387	ARG	CD-NE-CZ	-5.65	115.69	123.60
1	B	198	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	387	ARG	CB-CG-CD	5.57	126.09	111.60
1	B	312	GLU	O-C-N	5.48	131.52	121.10
1	A	152	GLU	N-CA-CB	5.39	120.30	110.60
1	B	177	GLU	N-CA-CB	-5.34	100.98	110.60
1	B	544	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	C	317	ARG	CG-CD-NE	5.30	122.93	111.80
1	A	387	ARG	CA-CB-CG	5.28	125.01	113.40
1	A	151	GLN	C-N-CA	-5.17	108.78	121.70
1	A	387	ARG	CG-CD-NE	-5.16	100.97	111.80
1	B	397	GLU	CA-CB-CG	5.07	124.56	113.40
1	B	317	ARG	CA-CB-CG	5.02	124.44	113.40

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	78	1
1	B	3194	0	3168	102	6
1	C	3194	0	3170	89	0
1	D	3194	0	3170	84	6
2	A	36	0	0	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	36	0	0	2	0
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	347	7

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 (347) 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: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:C:143:LEU:HD12	1:C:212:THR:HG22	1.62	0.82
1:A:202:LYS:HG2	1:A:202:LYS:O	1.81	0.80
1:C:189:THR:OG1	3:C:601:HOH:O	1.99	0.80
1:D:289:LYS:HD3	1:D:338:ALA:HB2	1.63	0.79
1:A:265:VAL:HG22	1:A:498:MET:HE2	1.62	0.79
1:B:205:GLN:HG2	1:B:205:GLN:O	1.80	0.79
1:B:250:ILE:HD11	1:B:253:LEU:HD13	1.65	0.78
1:B:315:GLY:C	1:B:317:ARG:H	1.87	0.77
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:O	1:C:181:MET:HG3	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:A:279:LYS:HA	1:A:423:THR:HB	1.73	0.70
1:D:175:LEU:HB3	1:D:179:MET:HE3	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:286:SER:HG	1:D:466:TYR:HH	1.39	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: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: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:D:175:LEU:O	1:D:179:MET:HE1	1.96	0.65
1:B:252:GLN:HB3	1:B:377:THR:HG22	1.78	0.65
1:C:195:LEU:HA	1:C:199:LEU:HD23	1.80	0.64
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:C:181:MET:SD	1:C:185:THR:HG23	2.38	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: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: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:A:251:PRO:HB2	1:A:255:LYS:HZ3	1.65	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:MET:HA	1:A:182:LEU:HD23	1.83	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: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:N	1:D:140:GLU:OE2	2.34	0.58
1:D:175:LEU:HB3	1:D:179:MET:CE	2.33	0.58
1:B:260:LEU:HD23	1:B:501:TRP:HH2	1.66	0.58
1:C:252:GLN:HE21	1:C:376:ALA:C	2.07	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
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: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:HD23	1:D:139:LEU:O	2.03	0.57
1:A:251:PRO:HB2	1:A:255:LYS:HZ2	1.69	0.57
1:A:289:LYS:HE3	1:A:338:ALA:CB	2.35	0.57
1:B:192:GLY:C	1:B:194:MET:H	2.07	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:318:PHE:C	1:B:320:LYS:H	2.09	0.55
1:C:427:ALA:O	1:C:430:MET:HB2	2.06	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:B:235:TYR:CE2	1:B:261:TRP:CD1	2.95	0.55
1:C:314:SER:HB2	1:C:318:PHE:CB	2.37	0.55
1:B:529:ASN:ND2	1:C:529:ASN:OD1	2.38	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
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:189:THR:OG1	1:D:191:ASP:OD1	2.11	0.54
1:D:216:ARG:HA	1:D:216:ARG:HE	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:A:250:ILE:HD12	1:A:252:GLN:HB2	1.90	0.53
1:D:175:LEU:O	1:D:179:MET:CE	2.56	0.53
1:C:316:LEU:HD11	1:C:467:ASP:CG	2.29	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: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: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: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
1:C:317:ARG:HH22	2:D:601:U27:C01	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:601:HOH:O	2.41	0.52
1:C:488:ILE:HD12	1:C:514:GLY:HA3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:315:GLY:C	1:B:317:ARG:N	2.62	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
1:C:317:ARG:NH2	2:D:601:U27:C01	2.75	0.50
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:B:293:TYR:OH	1:B:306:HIS:NE2	2.29	0.49
1:B:278:THR:HG22	1:B:425:GLU:HG2	1.92	0.49
1:A:317:ARG:HA	1:A:319:ASN:OD1	2.11	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:162:ALA:HB1	1:C:215:PHE:HE1	1.78	0.49
1:C:146:THR:HG21	1:C:216:ARG:HH21	1.77	0.49
1:D:143:LEU:HD12	1:D:212:THR:HG22	1.95	0.49
1:B:507:LYS:HG3	1:B:507:LYS:O	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:316:LEU:HD23	1:D:319:ASN:CG	2.33	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:SER:OG	1:C:278:THR:CG2	2.62	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:D:313:PRO:HG3	1:D:462:SER:HB2	1.95	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
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: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:C:422:VAL:CG1	1:C:430:MET:HE1	2.45	0.47
1:D:255:LYS:HG3	1:D:256:PHE:N	2.29	0.47
1:A:454:ARG:HD2	1:D:528:HIS:CG	2.50	0.47
1:A:322:PHE:O	1:A:323:LEU:HD23	2.15	0.47
1:D:329:PRO:HG2	1:D:340:VAL:HG21	1.97	0.46
1:B:527:PHE:CZ	1:B:542:PRO:HG2	2.49	0.46
1:C:422:VAL:HG11	1:C:430:MET:CE	2.45	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:C:377:THR:HG22	1:C:419:SER:HB3	1.97	0.45
1:D:147:ILE:O	3:D:701:HOH:O	2.20	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ARG:HB2	1:B:218:LYS:HG3	1.98	0.45
1:D:427:ALA:HA	1:D:430:MET:HE2	1.98	0.45
1:A:279:LYS:HZ2	1:A:426:SER:H	1.65	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
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:B:314:SER:C	1:B:317:ARG:NH1	2.70	0.45
1:A:423:THR:N	1:A:426:SER:OG	2.44	0.44
1:B:498:MET:HE3	1:B:498:MET:HB3	1.83	0.44
1:D:346:LYS:O	1:D:354:LYS:HE2	2.16	0.44
1:B:281:PRO:HA	1:B:422:VAL:O	2.17	0.44
1:B:252:GLN:CB	1:B:377:THR:HG22	2.45	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:C:318:PHE:C	1:C:320:LYS:H	2.20	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: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:C:422:VAL:HG11	1:C:430:MET:HE3	2.01	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ALA:HA	1:B:154:ILE:HG12	1.99	0.43
1:D:179:MET:HE2	1:D:179:MET:HB2	1.49	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
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:B:450:PRO:HG2	1:C:537:ALA:HB2	2.00	0.43
1:B:192:GLY:C	1:B:194:MET:N	2.72	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: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:B:498:MET:HE1	1:B:517:PHE:CE1	2.54	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:289:LYS:N	1:D:290:PRO:HD2	2.34	0.42
1:D:253:LEU:HD22	1:D:485:ALA:HA	2.00	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:B:318:PHE:C	1:B:320:LYS:N	2.73	0.42
1:B:391:ILE:HG22	1:B:395:LEU:HD11	2.01	0.42
1:B:252:GLN:N	1:B:252:GLN:OE1	2.51	0.42
1:B:317:ARG:HE	1:B:317:ARG:HB3	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:A:426:SER:HG	1:A:427:ALA:H	1.66	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: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:D:192:GLY:HA3	1:D:193:VAL:HA	1.72	0.42
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:PRO:HG3	1:B:462:SER:HB2	2.03	0.41
1:D:427:ALA:HA	1:D:430:MET:CE	2.50	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: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:C:332:PRO:HB2	1:C:333:MET:CE	2.51	0.41
1:D:289:LYS:HD3	1:D:338:ALA:CB	2.43	0.41
1:D:454:ARG:HD3	1:D:454:ARG:HH11	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:411:LEU:HD13	1:A:411:LEU:HA	1.78	0.41
1:B:332:PRO:CD	1:B:459:LEU:HD13	2.51	0.41
1:A:195:LEU:HD12	1:A:199:LEU:HG	2.03	0.41
1:B:225:MET:HB2	1:B:225:MET:HE3	1.99	0.41
1:B:250:ILE:HG13	1:B:253:LEU:H	1.86	0.41
1:D:139:LEU:HD23	1:D:139:LEU:C	2.40	0.41
1:D:410:ILE:HA	1:D:410:ILE:HD13	1.89	0.41
1:A:182:LEU:O	1:A:186:LEU:CD1	2.68	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:422:VAL:HG12	1:C:430:MET:HE1	2.03	0.40
1:B:426:SER:HG	1:B:427:ALA:H	1.69	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 (7) 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:601:U27:C26[4_445]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	47	69
1	C	408/527 (77%)	388 (95%)	19 (5%)	1 (0%)	47	69
1	D	408/527 (77%)	385 (94%)	21 (5%)	2 (0%)	29	47
All	All	1631/2108 (77%)	1547 (95%)	80 (5%)	4 (0%)	47	69

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%)	344 (98%)	9 (2%)	47	67
1	B	353/451 (78%)	341 (97%)	12 (3%)	37	58
1	C	353/451 (78%)	343 (97%)	10 (3%)	43	63
1	D	353/451 (78%)	340 (96%)	13 (4%)	34	54
All	All	1412/1804 (78%)	1368 (97%)	44 (3%)	40	60

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	ASP
1	A	217	ARG
1	A	249	TYR
1	A	286	SER
1	A	292	LYS
1	A	351	ASN
1	A	361	PHE
1	A	387	ARG
1	A	544	ARG
1	B	138	SER
1	B	178	CYS
1	B	186	LEU
1	B	264	SER
1	B	303	GLU
1	B	343	SER
1	B	361	PHE
1	B	374	SER
1	B	380	SER
1	B	384	SER
1	B	387	ARG
1	B	523	SER
1	C	194	MET
1	C	201	LYS
1	C	210	LEU
1	C	216	ARG
1	C	255	LYS
1	C	317	ARG
1	C	361	PHE
1	C	387	ARG
1	C	496	MET
1	C	524	LEU
1	D	138	SER
1	D	153	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	179	MET
1	D	196	ASP
1	D	237	SER
1	D	249	TYR
1	D	255	LYS
1	D	264	SER
1	D	319	ASN
1	D	343	SER
1	D	361	PHE
1	D	471	GLN
1	D	523	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	B	319	ASN
1	B	375	ASN
1	B	471	GLN
1	C	298	ASN
1	C	388	ASN
1	C	455	ASN
1	D	241	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	U27	A	601	1	32,40,40	3.19	18 (56%)	34,54,54	3.05	13 (38%)
2	U27	D	601	1	32,40,40	3.62	18 (56%)	34,54,54	2.93	14 (41%)

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	A	601	1	-	3/14/33/33	0/5/5/5
2	U27	D	601	1	-	2/14/33/33	0/5/5/5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	U27	C20-C21	7.68	1.64	1.51
2	D	601	U27	C12-N08	7.66	1.56	1.46
2	A	601	U27	C25-C24	7.60	1.58	1.38
2	D	601	U27	C07-N08	6.93	1.43	1.32
2	D	601	U27	C02-N03	6.59	1.50	1.35
2	A	601	U27	C02-N03	5.79	1.48	1.35
2	D	601	U27	C04-N03	5.53	1.46	1.36
2	A	601	U27	C19-N18	5.43	1.47	1.35
2	D	601	U27	C01-C31	5.40	1.60	1.51
2	D	601	U27	C19-N18	5.14	1.47	1.35
2	A	601	U27	C23-C24	4.76	1.50	1.38
2	A	601	U27	C25-C26	4.58	1.48	1.38
2	A	601	U27	C12-N08	4.54	1.52	1.46
2	D	601	U27	C17-N18	4.46	1.44	1.36
2	A	601	U27	C26-C21	4.33	1.48	1.38
2	A	601	U27	C07-N08	4.06	1.38	1.32
2	A	601	U27	C01-C02	3.99	1.60	1.51
2	D	601	U27	C01-C02	3.75	1.60	1.51
2	A	601	U27	C22-C21	3.73	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	U27	C01-C31	3.69	1.57	1.51
2	A	601	U27	C04-N03	3.41	1.42	1.36
2	D	601	U27	C36-C31	3.31	1.46	1.38
2	D	601	U27	C12-C11	2.90	1.57	1.52
2	A	601	U27	C20-C21	-2.85	1.47	1.51
2	D	601	U27	C22-C21	2.80	1.44	1.38
2	D	601	U27	C20-C19	2.76	1.58	1.51
2	A	601	U27	C35-C34	2.38	1.44	1.38
2	D	601	U27	C26-C21	2.32	1.43	1.38
2	A	601	U27	C34-C33	2.25	1.44	1.38
2	D	601	U27	C35-C34	2.24	1.44	1.38
2	A	601	U27	C36-C31	2.13	1.43	1.38
2	D	601	U27	C32-C31	2.10	1.43	1.38
2	A	601	U27	C23-C22	-2.08	1.34	1.38
2	A	601	U27	C12-C11	2.05	1.56	1.52
2	D	601	U27	C23-C24	2.03	1.43	1.38
2	D	601	U27	C35-C36	2.01	1.43	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	U27	C20-C19-N18	10.62	136.72	114.77
2	D	601	U27	C20-C19-N18	8.02	131.34	114.77
2	D	601	U27	C11-C12-N08	7.47	112.02	102.75
2	A	601	U27	O27-C19-C20	-6.94	106.24	122.03
2	D	601	U27	O27-C19-N18	-6.25	112.23	123.63
2	A	601	U27	C11-C12-N08	5.54	109.63	102.75
2	D	601	U27	C01-C02-N03	4.99	125.08	114.77
2	A	601	U27	C09-N08-C12	-4.15	100.83	111.55
2	D	601	U27	C10-C09-N08	4.07	108.13	103.35
2	D	601	U27	C09-N08-C12	-3.95	101.34	111.55
2	A	601	U27	C24-C25-C26	-3.67	114.59	120.19
2	A	601	U27	O27-C19-N18	-3.63	117.01	123.63
2	D	601	U27	C21-C20-C19	3.48	122.88	112.57
2	A	601	U27	C01-C02-N03	3.38	121.75	114.77
2	D	601	U27	O13-C11-C10	3.18	119.75	108.63
2	A	601	U27	C23-C22-C21	3.10	125.39	120.63
2	D	601	U27	O13-C11-C12	3.03	115.56	108.19
2	D	601	U27	O30-C02-N03	-2.85	118.44	123.63
2	A	601	U27	O13-C11-C12	2.67	114.69	108.19
2	A	601	U27	C10-C09-N08	2.56	106.35	103.35
2	D	601	U27	O27-C19-C20	-2.49	116.36	122.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	U27	C12-N08-C07	2.47	130.55	123.57
2	D	601	U27	O30-C02-C01	-2.44	116.48	122.03
2	A	601	U27	O13-C11-C10	2.40	117.00	108.63
2	A	601	U27	O30-C02-N03	-2.34	119.36	123.63
2	D	601	U27	C12-N08-C07	2.23	129.88	123.57
2	D	601	U27	C17-N18-C19	2.12	135.27	129.54

There are no chirality outliers.

All (5) torsion outliers are listed below:

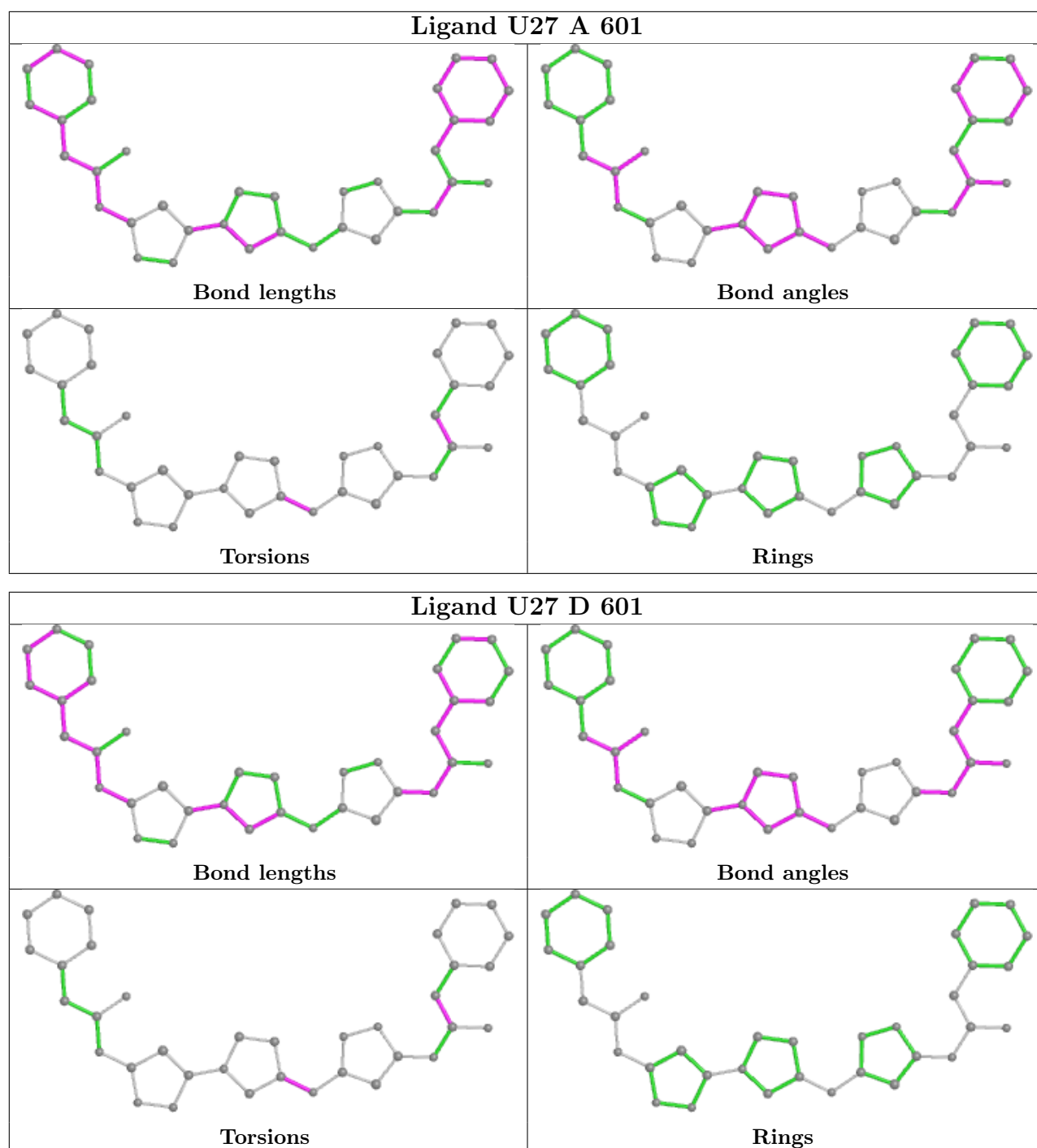
Mol	Chain	Res	Type	Atoms
2	A	601	U27	C12-C11-O13-C14
2	D	601	U27	C10-C11-O13-C14
2	A	601	U27	C10-C11-O13-C14
2	D	601	U27	O27-C19-C20-C21
2	A	601	U27	N18-C19-C20-C21

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	U27	0	1
2	D	601	U27	2	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%)	0.64	49 (11%) 4 4	45, 61, 116, 204	0
1	B	410/527 (77%)	0.71	47 (11%) 4 5	41, 59, 124, 218	0
1	C	410/527 (77%)	0.55	40 (9%) 7 8	41, 61, 115, 176	0
1	D	410/527 (77%)	0.51	33 (8%) 12 15	41, 58, 105, 188	0
All	All	1639/2108 (77%)	0.60	169 (10%) 6 7	41, 60, 116, 218	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	GLY	11.4
1	B	191	ASP	9.8
1	D	190	SER	9.1
1	B	189	THR	7.8
1	B	250	ILE	7.4
1	B	251	PRO	7.3
1	B	150	GLY	6.9
1	B	318	PHE	6.1
1	A	189	THR	5.9
1	D	318	PHE	5.7
1	C	193	VAL	5.7
1	B	193	VAL	5.6
1	B	252	GLN	5.4
1	B	148	ALA	5.4
1	D	144	PHE	5.3
1	A	145	TYR	5.3
1	A	149	GLU	5.3
1	A	191	ASP	5.2
1	A	150	GLY	5.2
1	B	188	THR	5.2
1	B	249	TYR	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	152	GLU	5.0
1	D	137	PRO	5.0
1	B	317	ARG	4.9
1	D	191	ASP	4.9
1	D	138	SER	4.9
1	C	191	ASP	4.9
1	D	193	VAL	4.8
1	A	251	PRO	4.8
1	A	148	ALA	4.7
1	D	208	ILE	4.6
1	A	154	ILE	4.6
1	A	200	PHE	4.6
1	A	193	VAL	4.5
1	B	192	GLY	4.4
1	B	145	TYR	4.3
1	A	188	THR	4.3
1	B	152	GLU	4.3
1	D	195	LEU	4.3
1	A	160	ILE	4.3
1	C	145	TYR	4.2
1	D	192	GLY	4.2
1	A	317	ARG	4.2
1	B	546	GLY	4.1
1	B	149	GLU	4.0
1	C	249	TYR	4.0
1	D	149	GLU	3.9
1	A	144	PHE	3.9
1	C	194	MET	3.8
1	A	156	VAL	3.8
1	B	258	PRO	3.8
1	B	167	GLY	3.7
1	C	192	GLY	3.7
1	A	228	THR	3.7
1	C	144	PHE	3.7
1	D	145	TYR	3.7
1	A	194	MET	3.7
1	A	143	LEU	3.7
1	D	200	PHE	3.7
1	C	252	GLN	3.7
1	D	148	ALA	3.6
1	C	190	SER	3.5
1	A	195	LEU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	252	GLN	3.5
1	B	200	PHE	3.5
1	B	147	ILE	3.4
1	B	160	ILE	3.4
1	C	251	PRO	3.4
1	A	250	ILE	3.3
1	B	137	PRO	3.3
1	A	153	LYS	3.3
1	A	186	LEU	3.3
1	B	186	LEU	3.3
1	A	146	THR	3.2
1	B	146	THR	3.2
1	C	138	SER	3.2
1	C	150	GLY	3.2
1	A	318	PHE	3.2
1	A	196	ASP	3.2
1	A	151	GLN	3.1
1	B	157	HIS	3.1
1	B	154	ILE	3.1
1	B	387	ARG	3.1
1	A	249	TYR	3.1
1	D	348	GLY	3.1
1	B	213	GLN	3.1
1	A	190	SER	3.0
1	C	152	GLU	3.0
1	A	376	ALA	3.0
1	B	151	GLN	3.0
1	B	197	LYS	3.0
1	D	158	LYS	3.0
1	D	397	GLU	3.0
1	C	318	PHE	2.9
1	A	372	GLY	2.9
1	B	254	ALA	2.9
1	B	205	GLN	2.9
1	B	144	PHE	2.9
1	D	194	MET	2.9
1	C	137	PRO	2.9
1	A	253	LEU	2.8
1	D	249	TYR	2.8
1	B	195	LEU	2.8
1	B	198	ASP	2.8
1	C	149	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	138	SER	2.7
1	D	206	SER	2.7
1	D	150	GLY	2.7
1	B	185	THR	2.7
1	A	141	ASP	2.7
1	B	169	ARG	2.7
1	A	213	GLN	2.7
1	C	256	PHE	2.7
1	A	137	PRO	2.6
1	D	151	GLN	2.6
1	C	154	ILE	2.6
1	D	188	THR	2.6
1	C	188	THR	2.6
1	C	148	ALA	2.6
1	A	279	LYS	2.5
1	B	187	GLN	2.5
1	D	160	ILE	2.5
1	C	157	HIS	2.5
1	C	387	ARG	2.5
1	B	256	PHE	2.5
1	C	200	PHE	2.5
1	A	215	PHE	2.5
1	A	138	SER	2.5
1	C	162	ALA	2.4
1	D	157	HIS	2.4
1	B	199	LEU	2.4
1	D	142	LEU	2.4
1	C	141	ASP	2.4
1	A	157	HIS	2.4
1	C	142	LEU	2.4
1	A	254	ALA	2.4
1	B	255	LYS	2.4
1	C	169	ARG	2.4
1	C	317	ARG	2.4
1	B	161	THR	2.4
1	D	152	GLU	2.4
1	A	155	PRO	2.3
1	C	187	GLN	2.3
1	B	153	LYS	2.3
1	C	147	ILE	2.3
1	D	255	LYS	2.3
1	D	156	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	181	MET	2.3
1	A	202	LYS	2.3
1	C	199	LEU	2.3
1	C	207	ASN	2.3
1	A	187	GLN	2.2
1	C	153	LYS	2.2
1	D	317	ARG	2.2
1	A	162	ALA	2.2
1	D	316	LEU	2.2
1	A	175	LEU	2.2
1	B	143	LEU	2.2
1	C	208	ILE	2.1
1	B	196	ASP	2.1
1	C	217	ARG	2.1
1	C	139	LEU	2.1
1	C	254	ALA	2.1
1	A	185	THR	2.1
1	A	147	ILE	2.1
1	C	216	ARG	2.1
1	C	375	ASN	2.1
1	D	496	MET	2.0
1	D	153	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	U27	A	601	36/36	0.90	0.32	56,103,168,176	0

Continued on next page...

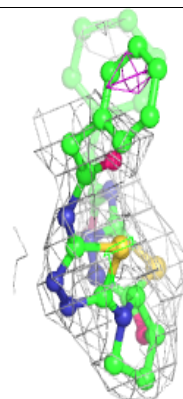
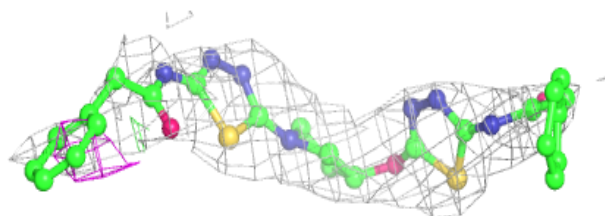
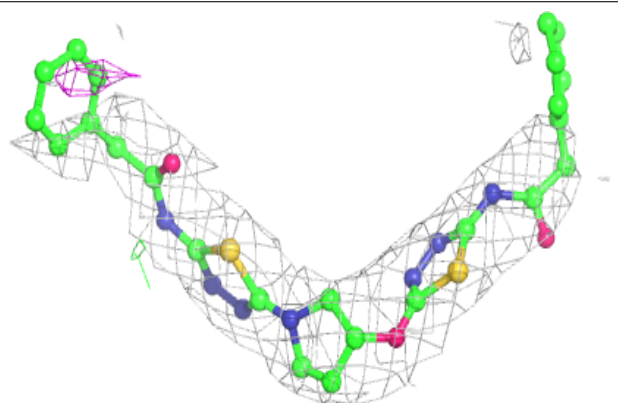
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	U27	D	601	36/36	0.90	0.30	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.

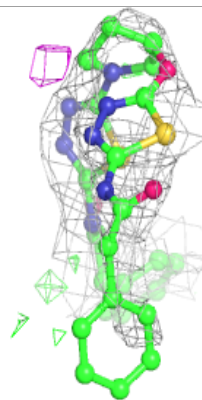
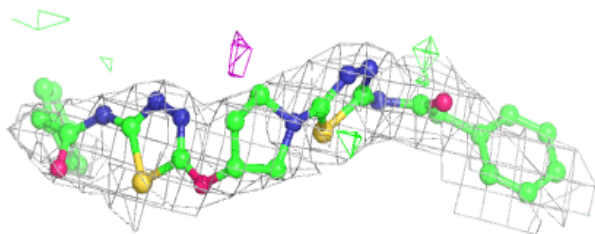
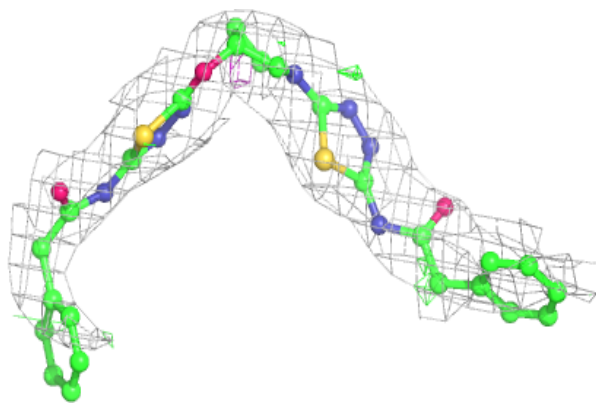
Electron density around U27 A 601:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around U27 D 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.