



# Full wwPDB X-ray Structure Validation Report i

Oct 18, 2022 – 01:21 pm BST

PDB ID : 7AIY

Title : Crystal structure of human butyrylcholinesterase in complex with 2-[1-[4-(12-Amino-3-chloro-6,7,10,11-tetrahydro-7,11-methanocycloocta[b]quinolin-9-yl)butyl]-1H-1,2,3-triazol-4-yl]-N-[4-hydroxy-3-methoxybenzyl]acetamide

Authors : Coquelle, N.; Colletier, J.P.

Deposited on : 2020-09-28

Resolution : 2.94 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](mailto: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 i symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.31.2

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0267

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001)

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.31.2

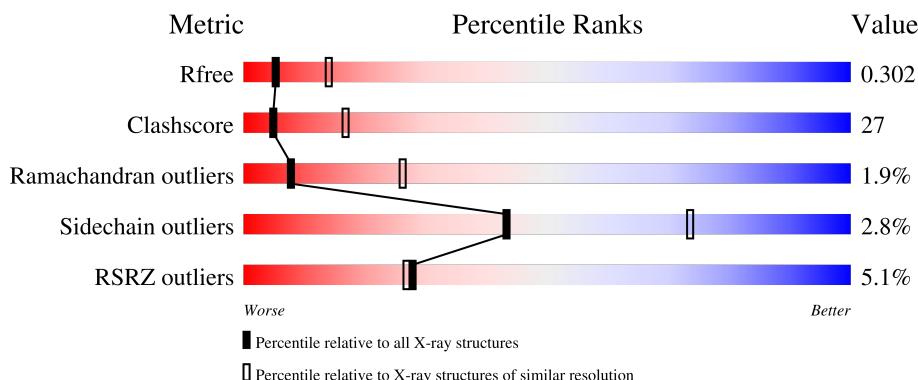
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

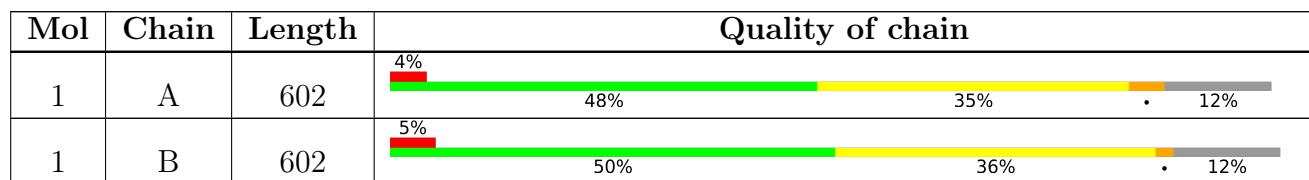
The reported resolution of this entry is 2.94 Å.

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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.



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	8U2	A	601	X	-	-	-

## 2 Entry composition [\(i\)](#)

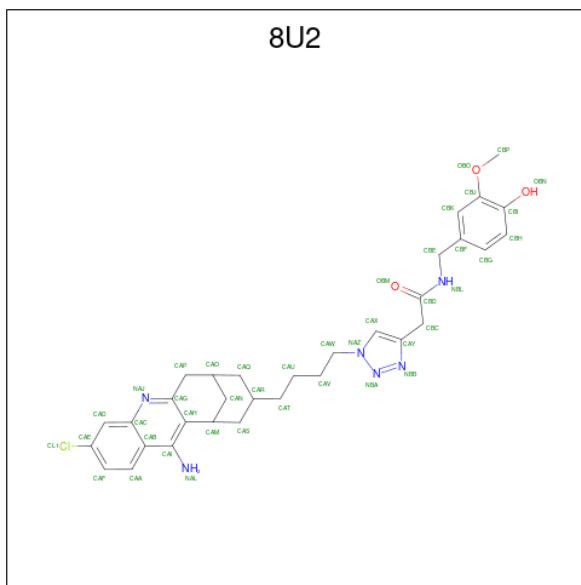
There are 2 unique types of molecules in this entry. The entry contains 8498 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cholinesterase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S		
			4228	2725	714	774	15	5	5
1	B	527	Total	C	N	O	S		
			4228	2725	714	774	15	5	5

- Molecule 2 is 2-{1-[4-(12-Amino-3-chloro-6,7,10,11-tetrahydro-7,11-methanocycloocta [b]quinolin-9-yl)butyl]-1H-1,2,3-triazol-4-yl}-N-[4-hydroxy-3-methoxybenzyl]acetamide (three-letter code: 8U2) (formula: C<sub>32</sub>H<sub>37</sub>ClN<sub>6</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).

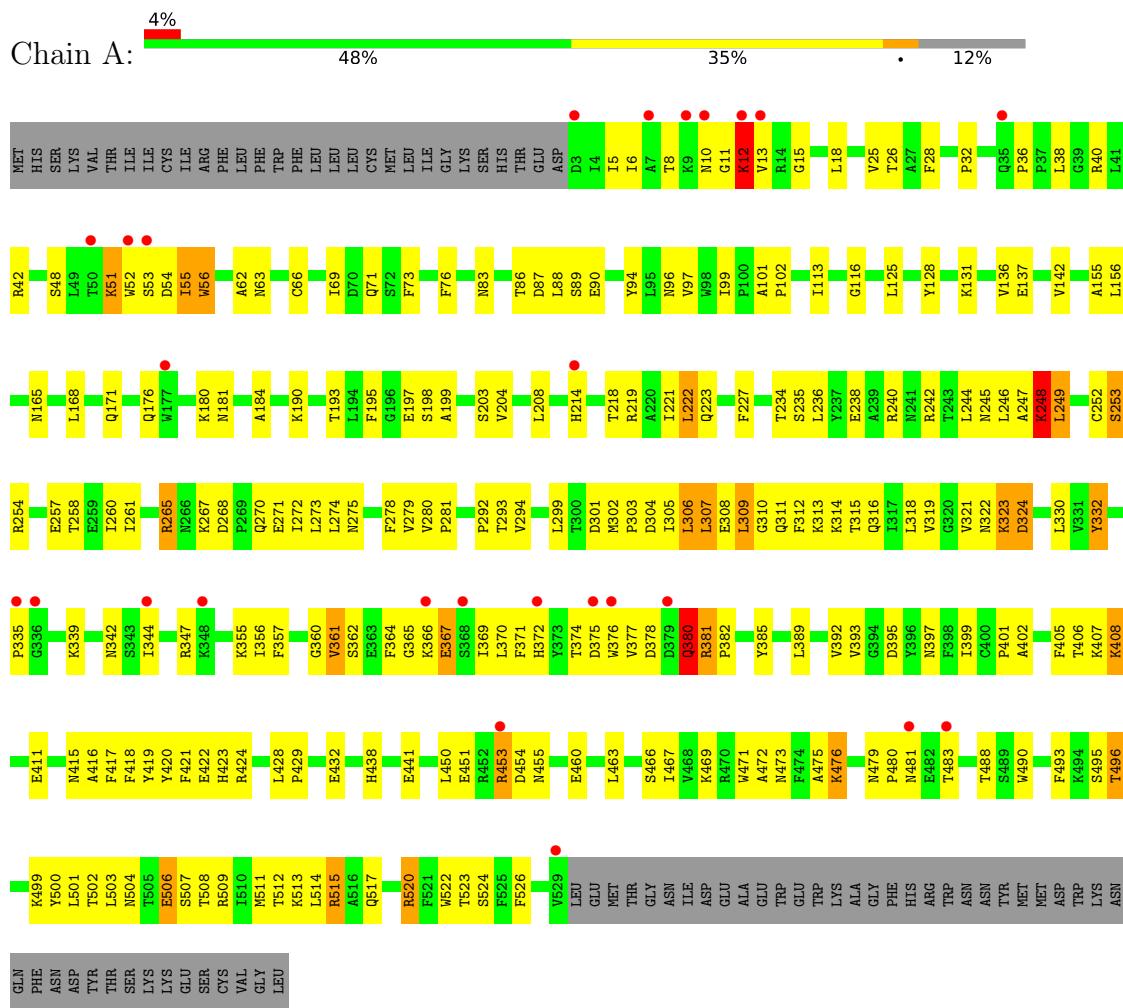


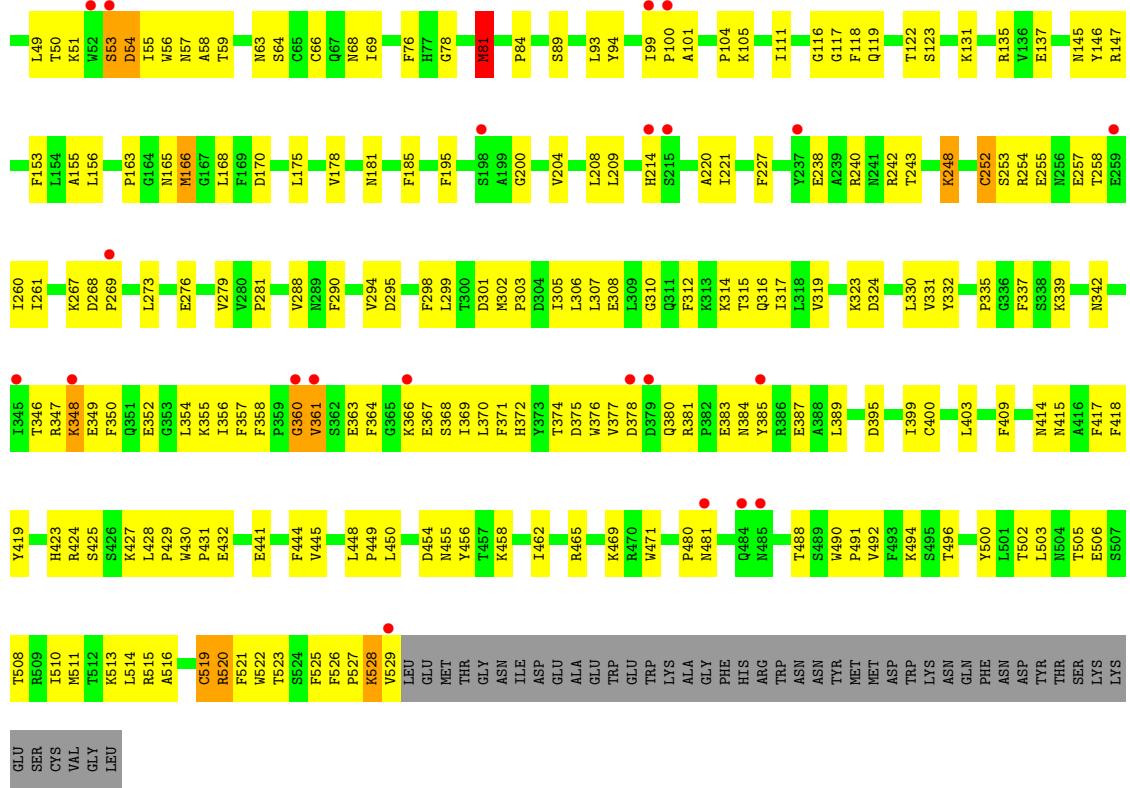
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	
			42	32	1	6	3	0

### 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: Cholinesterase





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.88Å    79.32Å    228.71Å 90.00°    90.00°    90.00°	Depositor
Resolution (Å)	48.87    –    2.94 48.87    –    2.94	Depositor EDS
% Data completeness (in resolution range)	91.3 (48.87-2.94) 81.1 (48.87-2.94)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	0.70 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
$R$ , $R_{free}$	0.225 , 0.300 0.231 , 0.302	Depositor DCC
$R_{free}$ test set	1358 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.2	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	8498	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 8U2

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	0.65	8/4357 (0.2%)	0.85	15/5918 (0.3%)
1	B	0.55	0/4357	0.77	7/5918 (0.1%)
All	All	0.60	8/8714 (0.1%)	0.81	22/11836 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	520	ARG	CZ-NH1	-9.12	1.21	1.33
1	A	520	ARG	NE-CZ	-8.76	1.21	1.33
1	A	520	ARG	CZ-NH2	-8.33	1.22	1.33
1	A	332	TYR	CE1-CZ	-7.22	1.29	1.38
1	A	56	TRP	CB-CG	-7.12	1.37	1.50
1	A	36	PRO	C-N	-6.99	1.21	1.34
1	A	520	ARG	CD-NE	-6.92	1.34	1.46
1	A	408	LYS	CB-CG	-5.24	1.38	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	ILE	CG1-CB-CG2	-12.80	83.24	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	LYS	CD-CE-NZ	11.38	137.87	111.70
1	A	222	LEU	CB-CG-CD2	-8.58	96.42	111.00
1	A	309	LEU	CA-CB-CG	7.63	132.84	115.30
1	B	520	ARG	NE-CZ-NH1	-7.29	116.66	120.30
1	A	307	LEU	CB-CG-CD1	-6.81	99.42	111.00
1	B	448	LEU	CA-CB-CG	6.69	130.69	115.30
1	A	306	LEU	CA-CB-CG	6.36	129.94	115.30
1	B	53	SER	C-N-CA	6.34	137.56	121.70
1	A	307	LEU	CA-CB-CG	6.31	129.81	115.30
1	A	408	LYS	CB-CG-CD	-6.22	95.42	111.60
1	A	380	GLN	C-N-CA	6.22	137.24	121.70
1	A	12	LYS	CA-CB-CG	5.95	126.48	113.40
1	B	519	CYS	CA-CB-SG	-5.95	103.30	114.00
1	A	307	LEU	CB-CA-C	5.89	121.39	110.20
1	A	249	LEU	CB-CG-CD1	-5.67	101.36	111.00
1	A	53	SER	C-N-CA	5.29	134.94	121.70
1	B	53	SER	N-CA-C	5.25	125.18	111.00
1	A	306	LEU	CB-CG-CD1	-5.13	102.29	111.00
1	B	267	LYS	C-N-CA	-5.11	108.94	121.70
1	B	360	GLY	C-N-CA	5.03	134.27	121.70
1	A	248	LYS	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	A	155	ALA	Peptide
1	B	155	ALA	Peptide
1	B	481	ASN	Peptide

## 5.2 Too-close contacts [\(i\)](#)

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	4228	0	4122	249	1
1	B	4228	0	4125	213	1
2	A	42	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8498	0	8247	459	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (459) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LEU:HD21	1:A:90:GLU:HB2	1.32	1.05
1:B:5:ILE:HD11	1:B:14:ARG:HA	1.37	1.05
1:B:428:LEU:HD23	1:B:430:TRP:H	1.18	1.04
1:B:369:ILE:HG22	1:B:521:PHE:CZ	1.93	1.02
1:B:369:ILE:HG22	1:B:521:PHE:HZ	1.24	0.96
1:A:361:VAL:HG12	1:A:366:LYS:NZ	1.82	0.93
1:B:5:ILE:CD1	1:B:14:ARG:HA	1.99	0.92
1:A:248:LYS:HD3	1:A:249:LEU:HD12	1.50	0.92
1:A:248:LYS:NZ	1:A:249:LEU:HD11	1.85	0.91
1:A:248:LYS:HZ3	1:A:249:LEU:HD11	1.34	0.91
1:A:506:GLU:CD	1:A:507:SER:H	1.75	0.89
1:B:53:SER:N	1:B:54:ASP:HB2	1.88	0.89
1:A:520:ARG:HA	1:A:523:THR:HG22	1.55	0.88
1:A:355:LYS:HE2	1:A:366:LYS:HE2	1.55	0.87
1:A:380:GLN:HG2	1:A:381:ARG:H	1.36	0.87
1:B:381:ARG:HH11	1:B:383:GLU:HB2	1.40	0.87
1:A:12:LYS:HD2	1:A:55:ILE:HG22	1.57	0.86
1:A:422:GLU:OE2	1:A:509:ARG:NH2	2.07	0.86
1:A:355:LYS:HE2	1:A:366:LYS:CD	2.06	0.85
1:B:361:VAL:O	1:B:366:LYS:NZ	2.10	0.84
1:B:360:GLY:HA2	1:B:361:VAL:O	1.77	0.84
1:B:376:TRP:HA	1:B:376:TRP:CE3	2.12	0.83
1:A:361:VAL:HG12	1:A:366:LYS:HZ1	1.44	0.82
1:A:323:LYS:HD2	1:A:420:TYR:CZ	2.15	0.81
1:A:355:LYS:HE2	1:A:366:LYS:CE	2.11	0.80
1:B:5:ILE:HD11	1:B:13:VAL:O	1.81	0.80
1:A:370:LEU:O	1:A:374:THR:HG23	1.82	0.79
1:A:8:THR:HG23	1:A:10:ASN:H	1.45	0.79
1:A:347:ARG:HB2	1:A:385:TYR:CZ	2.17	0.79
1:A:218:THR:O	1:A:315:THR:HG21	1.82	0.78
1:A:408:LYS:HA	1:A:411:GLU:HG3	1.64	0.77
1:A:476:LYS:H	1:A:476:LYS:HD2	1.50	0.77
1:B:354:LEU:HD22	1:B:369:ILE:HD11	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:LYS:CE	1:A:366:LYS:HE2	2.15	0.76
1:A:235:SER:OG	1:A:238:GLU:OE2	2.04	0.76
1:A:362:SER:O	1:A:366:LYS:NZ	2.18	0.76
1:A:13:VAL:HG22	1:A:56:TRP:HB3	1.67	0.75
1:A:323:LYS:HE3	1:A:422:GLU:HB3	1.67	0.75
1:B:5:ILE:HD11	1:B:14:ARG:CA	2.16	0.75
1:B:354:LEU:CD2	1:B:369:ILE:HD11	2.16	0.75
1:B:16:MET:CE	1:B:59:THR:HA	2.17	0.74
1:A:323:LYS:NZ	1:A:420:TYR:CD2	2.56	0.74
1:B:428:LEU:CD2	1:B:430:TRP:H	1.99	0.74
1:A:301:ASP:OD2	1:A:302:MET:N	2.20	0.74
1:A:380:GLN:HG2	1:A:381:ARG:N	2.02	0.73
1:A:380:GLN:CG	1:A:381:ARG:H	1.93	0.73
1:B:123:SER:OG	1:B:145:ASN:ND2	2.22	0.73
1:B:16:MET:HE1	1:B:59:THR:C	2.09	0.73
1:B:69:ILE:HD11	1:B:84:PRO:HD2	1.69	0.72
1:B:20:VAL:O	1:B:135:ARG:NH1	2.21	0.72
1:A:309:LEU:HD22	1:A:311:GLN:HG3	1.71	0.72
1:A:97:VAL:HG12	1:A:142:VAL:HG13	1.71	0.71
1:A:73:PHE:CE2	1:A:332:TYR:HE2	2.08	0.71
1:A:261:ILE:HG22	1:A:265:ARG:HH21	1.55	0.70
1:A:63:ASN:HA	1:A:86:THR:CG2	2.21	0.70
1:B:255:GLU:N	1:B:255:GLU:OE1	2.25	0.70
1:A:360:GLY:HA2	1:A:361:VAL:O	1.92	0.70
1:B:16:MET:HE1	1:B:59:THR:O	1.92	0.70
1:A:69:ILE:HG22	1:A:71:GLN:OE1	1.92	0.70
1:B:248:LYS:HD3	1:B:253:SER:CB	2.21	0.69
1:B:378:ASP:H	1:B:380:GLN:NE2	1.91	0.69
1:A:479:ASN:OD1	1:A:481:ASN:OD1	2.09	0.69
1:B:381:ARG:HB3	1:B:384:ASN:OD1	1.93	0.69
1:A:136:VAL:HG21	1:A:450:LEU:HD23	1.73	0.69
1:A:12:LYS:NZ	1:A:55:ILE:HG21	2.07	0.68
1:B:254:ARG:HB3	1:B:255:GLU:OE1	1.94	0.68
1:A:376:TRP:HA	1:A:376:TRP:CE3	2.28	0.68
1:A:248:LYS:HD3	1:A:249:LEU:CD1	2.24	0.68
1:A:62:ALA:O	1:A:86:THR:HG21	1.93	0.67
1:A:422:GLU:CD	1:A:509:ARG:HH22	1.97	0.67
1:B:380:GLN:HG2	1:B:381:ARG:N	2.09	0.67
1:A:361:VAL:HG12	1:A:366:LYS:HZ2	1.58	0.67
1:B:432:GLU:O	1:B:432:GLU:HG2	1.95	0.66
1:A:451:GLU:HG3	1:A:454:ASP:CG	2.15	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:TRP:HA	1:B:376:TRP:HE3	1.56	0.66
1:A:240:ARG:NH1	1:A:257:GLU:OE2	2.23	0.66
1:A:156:LEU:HD11	1:A:261:ILE:HD11	1.77	0.65
1:A:63:ASN:HA	1:A:86:THR:HG21	1.78	0.65
1:B:348:LYS:O	1:B:352:GLU:HG2	1.95	0.65
1:A:428:LEU:HD12	1:A:429:PRO:HD2	1.79	0.65
1:A:451:GLU:HG3	1:A:454:ASP:OD2	1.96	0.65
1:A:424:ARG:NH1	1:A:428:LEU:HD23	2.12	0.65
1:B:257:GLU:HA	1:B:260:ILE:HG12	1.79	0.64
1:A:479:ASN:OD1	1:A:481:ASN:CG	2.35	0.64
1:B:16:MET:HE1	1:B:59:THR:CA	2.28	0.64
1:A:15:GLY:HA3	1:A:28:PHE:CD2	2.33	0.63
1:B:12:LYS:HE3	1:B:55:ILE:HD12	1.78	0.63
1:A:253:SER:C	1:A:254:ARG:HD3	2.19	0.63
1:A:322:ASN:HD21	1:A:441:GLU:HG2	1.63	0.63
1:B:323:LYS:HG2	1:B:324:ASP:OD1	1.98	0.63
1:A:480:PRO:HB2	1:A:490:TRP:CE3	2.34	0.63
1:A:275:ASN:OD1	1:B:494:LYS:HE3	1.99	0.62
1:B:227:PHE:CE2	1:B:303:PRO:HB2	2.34	0.62
1:A:69:ILE:HD11	1:A:88:LEU:HD11	1.80	0.62
1:A:376:TRP:HA	1:A:376:TRP:HE3	1.65	0.62
1:A:323:LYS:HE3	1:A:422:GLU:CB	2.30	0.62
1:A:8:THR:HG22	1:A:11:GLY:O	1.99	0.61
1:A:323:LYS:HE3	1:A:422:GLU:CA	2.30	0.61
1:B:347:ARG:HG3	1:B:385:TYR:CE1	2.36	0.61
1:B:425:SER:OG	1:B:444:PHE:HE1	1.83	0.61
1:B:220:ALA:HB3	1:B:317:ILE:HG22	1.83	0.60
1:B:458:LYS:O	1:B:462:ILE:HD12	2.02	0.60
1:A:42:ARG:O	1:A:265:ARG:NH1	2.35	0.60
1:A:473:ASN:ND2	1:A:481:ASN:O	2.33	0.60
1:A:8:THR:OG1	1:A:181:ASN:OD1	2.19	0.60
1:A:38:LEU:HD21	1:A:90:GLU:CB	2.21	0.60
1:A:73:PHE:HE2	1:A:332:TYR:HE2	1.50	0.60
1:A:252:CYS:O	1:A:260:ILE:HD12	2.02	0.60
1:A:364:PHE:O	1:A:367:GLU:N	2.35	0.60
1:A:136:VAL:HG12	1:A:137:GLU:HG2	1.84	0.60
1:B:522:TRP:O	1:B:527:PRO:HD3	2.02	0.59
1:B:137:GLU:OE1	1:B:469:LYS:HD2	2.02	0.59
1:A:323:LYS:HD2	1:A:420:TYR:CE2	2.36	0.59
1:A:193:THR:HG21	1:A:475:ALA:HA	1.83	0.59
1:A:451:GLU:HG3	1:A:454:ASP:OD1	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:MET:HE2	1:B:59:THR:HA	1.84	0.59
1:A:422:GLU:HG3	1:A:504:ASN:HB3	1.84	0.59
1:A:12:LYS:NZ	1:A:55:ILE:CG2	2.66	0.59
1:A:463:LEU:O	1:A:466:SER:OG	2.21	0.59
1:A:5:ILE:HD11	1:A:12:LYS:HD3	1.85	0.59
1:B:395:ASP:OD1	1:B:515:ARG:NH2	2.37	0.58
1:A:236:LEU:HD21	1:A:294:VAL:O	2.02	0.58
1:B:294:VAL:HG21	1:B:302:MET:CE	2.34	0.58
1:A:249:LEU:HD12	1:A:249:LEU:H	1.67	0.58
1:A:355:LYS:NZ	1:A:366:LYS:HE2	2.18	0.58
1:B:43:PHE:O	1:B:166:MET:HE2	2.04	0.58
1:A:240:ARG:HH21	1:A:244:LEU:HD11	1.68	0.58
1:B:248:LYS:CD	1:B:253:SER:HB2	2.34	0.58
1:B:137:GLU:OE2	1:B:469:LYS:HE3	2.03	0.58
1:B:153:PHE:HE1	1:B:168:LEU:HD12	1.68	0.58
1:B:378:ASP:H	1:B:380:GLN:HE22	1.50	0.57
1:A:242:ARG:HA	1:A:245:ASN:HB2	1.86	0.57
1:B:301:ASP:OD2	1:B:302:MET:N	2.37	0.57
1:A:271:GLU:HA	1:B:415:ASN:HD21	1.69	0.57
1:B:428:LEU:HD23	1:B:430:TRP:N	2.02	0.56
1:A:271:GLU:O	1:A:275:ASN:ND2	2.38	0.56
1:B:16:MET:HE1	1:B:59:THR:HA	1.87	0.56
1:B:403:LEU:HD21	1:B:514:LEU:HD23	1.87	0.56
1:A:113:ILE:HD12	1:A:204:VAL:HG12	1.86	0.56
1:A:417:PHE:HB3	1:A:490:TRP:NE1	2.21	0.56
1:B:69:ILE:HD11	1:B:84:PRO:CD	2.36	0.56
1:B:200:GLY:O	1:B:204:VAL:HG23	2.05	0.56
1:B:314:LYS:HB3	1:B:414:ASN:HD21	1.70	0.56
1:B:361:VAL:HG13	1:B:366:LYS:HZ1	1.68	0.56
1:A:355:LYS:HE2	1:A:366:LYS:HD2	1.86	0.56
1:A:378:ASP:H	1:A:380:GLN:CD	2.09	0.56
1:B:68:ASN:OD1	1:B:273:LEU:HB3	2.06	0.56
1:B:441:GLU:O	1:B:445:VAL:HG23	2.06	0.56
1:B:454:ASP:O	1:B:455:ASN:HB2	2.05	0.56
1:B:5:ILE:HD11	1:B:13:VAL:C	2.26	0.56
1:B:248:LYS:CD	1:B:253:SER:CB	2.83	0.56
1:B:354:LEU:O	1:B:358:PHE:N	2.37	0.56
1:B:368:SER:O	1:B:372[B]:HIS:ND1	2.37	0.56
1:B:238:GLU:O	1:B:242:ARG:HG3	2.05	0.56
1:A:323:LYS:HZ1	1:A:420:TYR:C	2.09	0.56
1:B:111:ILE:HD11	1:B:178:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLN:O	1:A:274:LEU:HD12	2.06	0.55
1:A:234:THR:O	1:A:293:THR:HG22	2.05	0.55
1:B:528:LYS:HE3	1:B:529:VAL:HG13	1.88	0.55
1:B:4:ILE:HD12	1:B:4:ILE:O	2.07	0.55
1:B:380:GLN:HG2	1:B:381:ARG:H	1.70	0.55
1:A:156:LEU:HD22	1:A:257:GLU:HG2	1.89	0.55
1:A:12:LYS:CD	1:A:55:ILE:HG22	2.35	0.55
1:B:376:TRP:CZ2	1:B:384:ASN:HB3	2.42	0.55
1:B:399:ILE:HG22	1:B:403:LEU:HD11	1.88	0.55
1:A:301:ASP:O	1:A:306:LEU:HD11	2.05	0.55
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.41	0.55
1:A:309:LEU:O	1:A:309:LEU:HD23	2.07	0.54
1:A:319:VAL:HG11	1:A:406:THR:HB	1.88	0.54
1:A:402:ALA:O	1:A:406:THR:HG22	2.07	0.54
1:A:18:LEU:HB2	1:A:25:VAL:HG12	1.90	0.54
1:A:227:PHE:CE2	1:A:303:PRO:HB2	2.43	0.54
1:A:12:LYS:HZ1	1:A:55:ILE:HG21	1.71	0.54
1:A:245:ASN:O	1:A:248:LYS:N	2.34	0.54
1:B:14:ARG:O	1:B:58:ALA:N	2.41	0.54
1:B:425:SER:HG	1:B:444:PHE:HE1	1.55	0.54
1:B:66:CYS:HB3	1:B:273:LEU:HD11	1.90	0.54
1:A:40:ARG:O	1:A:265:ARG:NH1	2.41	0.54
1:B:21:PHE:C	1:B:135:ARG:HH12	2.10	0.54
1:B:319:VAL:O	1:B:418:PHE:HA	2.08	0.54
1:A:171:GLN:HE22	1:A:203:SER:HB3	1.73	0.54
1:A:248:LYS:CE	1:A:249:LEU:HD11	2.38	0.54
1:B:331:VAL:HG23	1:B:332:TYR:CD1	2.43	0.54
1:A:411:GLU:OE1	1:A:495:SER:OG	2.13	0.53
1:B:16:MET:CE	1:B:59:THR:CA	2.85	0.53
1:A:260:ILE:HG22	1:A:261:ILE:HG12	1.90	0.53
1:A:227:PHE:CZ	1:A:307:LEU:HD22	2.43	0.53
1:A:481:ASN:HB3	1:A:483:THR:HG23	1.89	0.53
1:A:12:LYS:HZ2	1:A:55:ILE:HG21	1.74	0.53
1:B:76:PHE:CE1	1:B:339:LYS:HD2	2.43	0.53
1:B:117:GLY:O	1:B:288:VAL:HG13	2.08	0.53
1:B:123:SER:H	1:B:145:ASN:HD21	1.56	0.53
1:B:350:PHE:CE2	1:B:354:LEU:HD11	2.44	0.53
1:B:352:GLU:O	1:B:356:ILE:HD12	2.09	0.53
1:A:323:LYS:HB2	1:A:324:ASP:OD1	2.08	0.53
1:A:254:ARG:H	1:A:260:ILE:HD13	1.74	0.52
1:A:323:LYS:NZ	1:A:420:TYR:C	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:ILE:CD1	1:B:13:VAL:O	2.56	0.52
1:B:500:TYR:CZ	1:B:511:MET:HB2	2.44	0.52
1:A:254:ARG:H	1:A:260:ILE:CD1	2.22	0.52
1:B:248:LYS:HD2	1:B:253:SER:HB2	1.92	0.52
1:A:5:ILE:HD11	1:A:12:LYS:NZ	2.25	0.52
1:A:513:LYS:CG	1:A:513:LYS:O	2.57	0.52
1:A:249:LEU:HD12	1:A:249:LEU:N	2.24	0.52
1:B:24:THR:HG23	1:B:101:ALA:HB3	1.91	0.52
1:B:163:PRO:HD2	1:B:166:MET:CE	2.40	0.52
1:B:165:ASN:HD22	1:B:295:ASP:CG	2.13	0.52
1:B:78:GLY:HA2	1:B:81:MET:CE	2.40	0.51
1:B:423:HIS:ND1	1:B:505:THR:HG23	2.25	0.51
1:B:254:ARG:HB2	1:B:260:ILE:HG23	1.93	0.51
1:B:513:LYS:HB3	1:B:516:ALA:HB2	1.93	0.51
1:A:268:ASP:OD1	1:A:271:GLU:HG2	2.11	0.51
1:A:369:ILE:HD11	1:A:526:PHE:CE1	2.45	0.51
1:A:323:LYS:HE2	1:A:421:PHE:C	2.31	0.51
1:A:245:ASN:O	1:A:246:LEU:C	2.49	0.51
1:A:208:LEU:O	1:A:214[B]:HIS:NE2	2.41	0.51
1:B:528:LYS:HD2	1:B:528:LYS:C	2.31	0.51
1:A:245:ASN:HB3	1:A:248:LYS:NZ	2.25	0.51
1:A:323:LYS:HE3	1:A:422:GLU:HA	1.92	0.51
1:B:14:ARG:HD2	1:B:57:ASN:OD1	2.10	0.51
1:A:274:LEU:HD22	1:B:492:VAL:HG13	1.93	0.50
1:A:321:VAL:HG21	1:A:399:ILE:HG12	1.92	0.50
1:A:73:PHE:HE2	1:A:332:TYR:CE2	2.29	0.50
1:A:176[B]:GLN:OE1	1:A:180:LYS:NZ	2.34	0.50
1:B:69:ILE:HD11	1:B:84:PRO:HG2	1.93	0.50
1:A:12:LYS:HZ2	1:A:55:ILE:CG2	2.25	0.50
1:A:197:GLU:HG3	1:A:441:GLU:OE2	2.11	0.50
1:A:245:ASN:O	1:A:248:LYS:HD2	2.12	0.50
1:B:8:THR:OG1	1:B:11:GLY:O	2.22	0.50
1:B:76:PHE:HZ	1:B:429:PRO:O	1.94	0.50
1:B:268:ASP:HB2	1:B:269:PRO:HD2	1.92	0.50
1:B:16:MET:CE	1:B:59:THR:OG1	2.59	0.50
1:B:417:PHE:HB3	1:B:490:TRP:NE1	2.26	0.50
1:B:424:ARG:NH2	1:B:432:GLU:HA	2.27	0.50
1:B:523:THR:O	1:B:527:PRO:HG3	2.12	0.50
1:A:501:LEU:HD11	1:A:508:THR:HB	1.94	0.50
1:B:69:ILE:CD1	1:B:84:PRO:HD2	2.40	0.50
1:A:438:HIS:NE2	2:A:601:8U2:NAL	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLY:HA3	1:A:28:PHE:HD2	1.74	0.50
1:A:330:LEU:HD23	1:A:357:PHE:CZ	2.47	0.50
1:A:506:GLU:OE1	1:A:507:SER:N	2.45	0.49
1:B:331:VAL:HG23	1:B:332:TYR:HD1	1.76	0.49
1:A:332:TYR:CD1	2:A:601:8U2:NBB	2.80	0.49
1:A:371:PHE:O	1:A:375[B]:ASP:OD1	2.30	0.49
1:B:25:VAL:HG11	1:B:131:LYS:HB2	1.94	0.49
1:B:376:TRP:HB3	1:B:378:ASP:C	2.33	0.49
1:B:424:ARG:NH2	1:B:430:TRP:O	2.38	0.49
1:A:15:GLY:HA3	1:A:28:PHE:CE2	2.46	0.49
1:A:306:LEU:HD12	1:A:306:LEU:H	1.77	0.49
1:B:342:ASN:N	1:B:342:ASN:OD1	2.45	0.49
1:B:480:PRO:HB2	1:B:490:TRP:CE3	2.47	0.49
1:A:42:ARG:NH2	1:A:272:ILE:HD12	2.28	0.49
1:B:307:LEU:HD12	1:B:312:PHE:CE2	2.48	0.49
1:B:491:PRO:HD3	1:B:510:ILE:HD12	1.95	0.49
1:A:502:THR:OG1	1:A:509:ARG:NH2	2.46	0.49
1:B:123:SER:H	1:B:145:ASN:ND2	2.11	0.49
1:A:319:VAL:O	1:A:418:PHE:HA	2.13	0.48
1:B:209:LEU:HD23	1:B:312:PHE:HB3	1.95	0.48
1:B:252:CYS:O	1:B:260:ILE:HG22	2.13	0.48
1:B:9:LYS:HD3	1:B:181:ASN:OD1	2.13	0.48
1:A:254:ARG:HD3	1:A:254:ARG:N	2.27	0.48
1:A:376:TRP:HB3	1:A:378:ASP:C	2.33	0.48
1:B:12:LYS:HZ2	1:B:55:ILE:HB	1.78	0.48
1:A:495:SER:O	1:A:496:THR:OG1	2.19	0.48
1:B:78:GLY:HA2	1:B:81:MET:HE3	1.95	0.48
1:B:352:GLU:HA	1:B:355:LYS:HE3	1.94	0.48
1:A:222:LEU:O	1:A:319:VAL:HA	2.13	0.48
1:B:240:ARG:HA	1:B:243:THR:HG22	1.96	0.48
1:B:399:ILE:O	1:B:403:LEU:HD12	2.13	0.48
1:A:393:VAL:O	1:A:397:ASN:ND2	2.38	0.48
1:A:401:PRO:O	1:A:405:PHE:N	2.42	0.48
1:A:5:ILE:HD11	1:A:12:LYS:HZ2	1.77	0.48
1:A:219:ARG:HA	1:A:315:THR:HG21	1.96	0.47
1:B:14:ARG:N	1:B:56:TRP:O	2.34	0.47
1:B:294:VAL:HG21	1:B:302:MET:HE1	1.96	0.47
1:A:26:THR:OG1	1:A:99:ILE:HB	2.14	0.47
1:B:16:MET:HG3	1:B:59:THR:OG1	2.14	0.47
1:B:208:LEU:O	1:B:214[B]:HIS:NE2	2.39	0.47
1:B:519:CYS:O	1:B:523:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:GLY:O	1:A:369:ILE:HG13	2.14	0.47
1:B:63:ASN:HB3	1:B:89:SER:HB3	1.96	0.47
1:A:378:ASP:H	1:A:380:GLN:NE2	2.12	0.47
1:B:100:PRO:HD2	1:B:104:PRO:HG2	1.96	0.47
1:A:240:ARG:NH2	1:A:244:LEU:HD11	2.28	0.47
1:A:407:LYS:HA	1:A:493:PHE:HE1	1.79	0.47
1:A:227:PHE:HZ	1:A:307:LEU:HD22	1.80	0.47
1:A:453:ARG:O	1:A:453:ARG:NE	2.47	0.47
1:B:258:THR:O	1:B:261:ILE:HG13	2.15	0.47
1:B:381:ARG:HH12	1:B:387:GLU:CD	2.18	0.47
1:A:15:GLY:CA	1:A:28:PHE:HD2	2.28	0.47
1:A:335:PRO:HD3	1:A:356:ILE:HD12	1.97	0.47
1:A:258:THR:O	1:A:258:THR:OG1	2.30	0.47
1:A:315:THR:HG23	1:A:316:GLN:OE1	2.15	0.47
1:B:317:ILE:HG12	1:B:409:PHE:CE2	2.50	0.47
1:B:361:VAL:HG13	1:B:366:LYS:NZ	2.29	0.47
1:B:377:VAL:HG22	1:B:377:VAL:O	2.14	0.47
1:B:13:VAL:HG21	1:B:31:ILE:HG12	1.97	0.47
1:B:381:ARG:NE	1:B:383:GLU:OE2	2.48	0.46
1:B:430:TRP:HB3	1:B:431:PRO:HD2	1.96	0.46
1:A:198:SER:OG	1:A:199:ALA:N	2.49	0.46
1:A:504:ASN:ND2	1:A:509:ARG:NH2	2.63	0.46
1:B:315:THR:OG1	1:B:316:GLN:N	2.49	0.46
1:A:261:ILE:HG22	1:A:265:ARG:NH2	2.27	0.46
1:B:502:THR:O	1:B:503:LEU:HD23	2.15	0.46
1:A:125:LEU:HD12	1:A:128:TYR:CE2	2.51	0.46
1:A:504:ASN:OD1	1:A:506:GLU:HG3	2.15	0.46
1:B:276:GLU:O	1:B:279:VAL:HG12	2.15	0.46
1:A:197:GLU:HA	1:A:223:GLN:O	2.16	0.46
1:A:454:ASP:O	1:A:455:ASN:HB2	2.16	0.46
1:B:156:LEU:HD13	1:B:257:GLU:HG3	1.97	0.46
1:A:355:LYS:HZ1	1:A:366:LYS:HE2	1.80	0.46
1:A:10:ASN:HB3	1:A:51:LYS:HA	1.98	0.45
1:A:25:VAL:HG11	1:A:131:LYS:HB2	1.98	0.45
1:A:195:PHE:CB	1:A:221:ILE:HB	2.46	0.45
1:A:347:ARG:NH1	1:A:370:LEU:HD21	2.30	0.45
1:A:406:THR:HG21	1:A:418:PHE:HD2	1.82	0.45
1:B:337:PHE:HE1	1:B:389:LEU:HD23	1.80	0.45
1:B:403:LEU:HD21	1:B:514:LEU:HB3	1.98	0.45
1:B:346:THR:OG1	1:B:347:ARG:N	2.50	0.45
1:A:421:PHE:HA	1:A:503:LEU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ARG:O	1:A:524:SER:OG	2.20	0.45
1:A:156:LEU:CD1	1:A:261:ILE:HD11	2.45	0.45
1:A:315:THR:CG2	1:A:316:GLN:N	2.80	0.45
1:B:330:LEU:HD23	1:B:357:PHE:CZ	2.52	0.45
1:A:66:CYS:HB3	1:A:273:LEU:HD11	1.98	0.45
1:A:424:ARG:NE	1:A:432:GLU:OE1	2.49	0.45
1:A:307:LEU:C	1:A:408:LYS:CE	2.85	0.45
1:A:370:LEU:O	1:A:371:PHE:C	2.55	0.45
1:B:99:ILE:HG21	1:B:185:PHE:HB3	1.98	0.45
1:B:295:ASP:OD1	1:B:295:ASP:N	2.50	0.45
1:A:302:MET:HG3	1:A:304:ASP:OD1	2.16	0.45
1:A:476:LYS:HD2	1:A:476:LYS:N	2.25	0.45
1:A:342:ASN:OD1	1:A:342:ASN:N	2.48	0.45
1:A:499:LYS:HG3	1:A:512:THR:HG22	1.98	0.45
1:B:339:LYS:HB3	1:B:339:LYS:HE3	1.56	0.45
1:A:305:ILE:HG13	1:A:306:LEU:N	2.32	0.44
1:B:347:ARG:HH11	1:B:370:LEU:HD21	1.82	0.44
1:B:5:ILE:HA	1:B:5:ILE:HD12	1.36	0.44
1:B:253:SER:C	1:B:254:ARG:HG2	2.38	0.44
1:B:450:LEU:HD21	1:B:465:ARG:HB2	1.99	0.44
1:A:323:LYS:CD	1:A:420:TYR:CZ	2.95	0.44
1:A:342:ASN:ND2	1:A:344:ILE:HG12	2.32	0.44
1:A:372[A]:HIS:CE1	1:A:517:GLN:HE21	2.35	0.44
1:A:323:LYS:N	1:A:323:LYS:HD3	2.33	0.44
1:B:156:LEU:HD23	1:B:243:THR:HG21	1.98	0.44
1:A:299:LEU:HD12	1:A:299:LEU:HA	1.82	0.44
1:B:12:LYS:HZ1	1:B:54:ASP:C	2.20	0.44
1:B:175:LEU:O	1:B:178:VAL:HG22	2.18	0.44
1:B:242:ARG:HB3	1:B:279:VAL:HG22	1.99	0.44
1:A:32:PRO:HB3	1:A:94:TYR:CE2	2.52	0.44
1:A:261:ILE:HD13	1:A:261:ILE:HA	1.73	0.44
1:A:12:LYS:HD2	1:A:55:ILE:CG2	2.39	0.44
1:B:195:PHE:CB	1:B:221:ILE:HB	2.48	0.44
1:B:335:PRO:HD2	1:B:356:ILE:HD13	1.98	0.44
1:B:449:PRO:HA	1:B:456:TYR:CD1	2.53	0.44
1:A:227:PHE:CD2	1:A:303:PRO:HB2	2.52	0.44
1:B:417:PHE:HB3	1:B:490:TRP:CE2	2.52	0.44
1:B:525:PHE:CD1	1:B:525:PHE:C	2.91	0.44
1:A:376:TRP:C	1:A:378:ASP:HA	2.38	0.44
1:A:309:LEU:CD2	1:A:311:GLN:HG3	2.43	0.43
1:B:69:ILE:HD11	1:B:84:PRO:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ILE:HG23	1:A:83:ASN:CG	2.38	0.43
1:A:245:ASN:O	1:A:248:LYS:CD	2.66	0.43
1:A:364:PHE:O	1:A:365:GLY:C	2.57	0.43
1:A:408:LYS:O	1:A:408:LYS:HG2	2.17	0.43
1:B:279:VAL:HG11	1:B:290:PHE:CE1	2.53	0.43
1:B:302:MET:HB2	1:B:305:ILE:HD12	2.01	0.43
1:B:310:GLY:HA2	1:B:312:PHE:CE2	2.54	0.43
1:B:462:ILE:HD12	1:B:462:ILE:H	1.83	0.43
1:A:310:GLY:HA2	1:A:312:PHE:CE2	2.53	0.43
1:A:312:PHE:HD1	1:A:313:LYS:O	2.01	0.43
1:B:146:TYR:HB2	1:B:170:ASP:HB2	2.01	0.43
1:B:163:PRO:HD2	1:B:166:MET:HE3	1.98	0.43
1:A:242:ARG:HD2	1:A:279:VAL:HG23	2.01	0.43
1:B:76:PHE:CZ	1:B:429:PRO:O	2.71	0.43
1:B:335:PRO:HB2	1:B:349:GLU:HB3	2.01	0.43
1:B:526:PHE:N	1:B:527:PRO:HD2	2.34	0.43
1:B:299:LEU:HD23	1:B:299:LEU:HA	1.79	0.43
1:A:419:TYR:OH	1:A:441:GLU:OE1	2.35	0.42
1:B:33:TYR:OH	1:B:170:ASP:HB3	2.18	0.42
1:B:227:PHE:CD2	1:B:303:PRO:HB2	2.54	0.42
1:B:308:GLU:O	1:B:308:GLU:HG2	2.19	0.42
1:B:525:PHE:C	1:B:527:PRO:HD2	2.39	0.42
1:A:222:LEU:HB2	1:A:319:VAL:HB	2.02	0.42
1:A:469:LYS:O	1:A:472:ALA:HB3	2.19	0.42
1:A:514:LEU:HD12	1:A:515:ARG:HG3	1.99	0.42
1:B:53:SER:CA	1:B:54:ASP:HB2	2.49	0.42
1:A:389:LEU:HA	1:A:392:VAL:HG22	2.01	0.42
1:A:420:TYR:CD1	1:A:514:LEU:HD21	2.54	0.42
1:B:21:PHE:HB2	1:B:135:ARG:NH1	2.34	0.42
1:B:364:PHE:O	1:B:367:GLU:N	2.47	0.42
1:A:6:ILE:HD11	1:A:184:ALA:O	2.19	0.42
1:B:69:ILE:HD13	1:B:69:ILE:HA	1.74	0.42
1:B:368:SER:O	1:B:371:PHE:HB3	2.19	0.42
1:A:302:MET:O	1:A:305:ILE:HG12	2.19	0.42
2:A:601:8U2:CAG	2:A:601:8U2:CAX	2.98	0.42
1:A:71:GLN:OE1	1:A:71:GLN:N	2.53	0.42
1:A:101:ALA:HA	1:A:102:PRO:C	2.38	0.42
1:A:377:VAL:C	1:A:380:GLN:HE22	2.23	0.42
1:B:146:TYR:HD1	1:B:147:ARG:O	2.02	0.42
1:B:294:VAL:HG21	1:B:302:MET:HE2	2.00	0.42
1:B:400:CYS:HA	1:B:403:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:LYS:HE3	1:B:462:ILE:HD11	2.02	0.42
1:A:395:ASP:HA	1:A:399:ILE:HB	2.02	0.42
1:B:168:LEU:HD22	1:B:298:PHE:CE1	2.55	0.42
1:A:332:TYR:CE1	2:A:601:8U2:NBB	2.88	0.42
1:A:513:LYS:O	1:A:513:LYS:HG2	2.19	0.42
1:A:378:ASP:N	1:A:380:GLN:HE22	2.18	0.42
1:B:105:LYS:HA	1:B:105:LYS:HD3	1.74	0.42
1:B:330:LEU:HD13	1:B:337:PHE:CZ	2.55	0.42
1:B:354:LEU:HD21	1:B:369:ILE:HD11	1.98	0.41
1:B:377:VAL:N	1:B:378:ASP:HA	2.35	0.41
1:A:278:PHE:C	1:A:280:VAL:H	2.22	0.41
1:B:117:GLY:O	1:B:119:GLN:HG2	2.20	0.41
1:B:32:PRO:HG3	1:B:94:TYR:CE2	2.55	0.41
1:B:248:LYS:HD3	1:B:253:SER:HB2	1.95	0.41
1:B:370:LEU:O	1:B:374:THR:HG22	2.19	0.41
1:A:378:ASP:C	1:A:380:GLN:H	2.24	0.41
1:A:381:ARG:HA	1:A:382:PRO:HD3	1.89	0.41
1:A:423:HIS:NE2	1:A:460:GLU:OE2	2.41	0.41
1:A:520:ARG:HH21	1:A:520:ARG:HD2	1.59	0.41
1:B:49:LEU:HD12	1:B:50:THR:H	1.84	0.41
1:B:419:TYR:CD2	1:B:419:TYR:C	2.94	0.41
1:A:28:PHE:HD1	1:A:97:VAL:CG2	2.33	0.41
1:A:38:LEU:HD23	1:A:38:LEU:HA	1.65	0.41
1:A:86:THR:CG2	1:A:87:ASP:N	2.84	0.41
1:A:165:ASN:OD1	1:A:292:PRO:HA	2.20	0.41
1:A:245:ASN:HA	1:A:248:LYS:HD2	2.02	0.41
1:B:369:ILE:HG22	1:B:521:PHE:CE2	2.48	0.41
1:B:491:PRO:HD3	1:B:510:ILE:CD1	2.51	0.41
1:B:526:PHE:O	1:B:529:VAL:HG22	2.20	0.41
1:B:303:PRO:HA	1:B:306:LEU:HD13	2.03	0.41
1:B:350:PHE:CD2	1:B:370:LEU:HD12	2.55	0.41
1:A:316:GLN:HA	1:A:415:ASN:O	2.20	0.41
1:A:323:LYS:HE2	1:A:421:PHE:O	2.21	0.41
1:B:37:PRO:C	1:B:38:LEU:HD23	2.42	0.41
1:A:267:LYS:HE2	1:A:267:LYS:HA	2.03	0.41
1:A:271:GLU:CA	1:B:415:ASN:HD21	2.32	0.41
1:A:374:THR:O	1:A:376:TRP:N	2.54	0.41
1:B:64:SER:HB3	1:B:122:THR:OG1	2.21	0.41
1:A:13:VAL:HG23	1:A:52:TRP:HZ2	1.86	0.41
1:A:332:TYR:HD1	2:A:601:8U2:NBB	2.19	0.41
1:A:416:ALA:O	1:A:493:PHE:N	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ILE:HD11	1:B:15:GLY:C	2.42	0.41
1:B:93:LEU:HD21	1:B:147:ARG:HG3	2.03	0.41
1:B:209:LEU:CD2	1:B:312:PHE:HB3	2.51	0.41
1:A:195:PHE:HB3	1:A:221:ILE:HB	2.02	0.40
1:A:247:ALA:HB1	1:A:260:ILE:HD11	2.03	0.40
1:A:76:PHE:CZ	1:A:339:LYS:HD2	2.55	0.40
1:A:406:THR:HG21	1:A:418:PHE:CD2	2.56	0.40
1:A:467:ILE:HG23	1:A:471:TRP:CZ3	2.56	0.40
1:A:312:PHE:O	1:A:314:LYS:HE3	2.21	0.40
1:B:376:TRP:CH2	1:B:384:ASN:HB3	2.56	0.40
1:B:488:THR:HG21	1:B:508:THR:O	2.21	0.40
1:A:369:ILE:HD13	1:A:522:TRP:HH2	1.86	0.40
1:B:306:LEU:H	1:B:306:LEU:HD12	1.87	0.40
1:A:318:LEU:HD11	1:A:490:TRP:CH2	2.57	0.40
1:B:56:TRP:CD1	1:B:56:TRP:C	2.94	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ARG:NH1	1:B:375[B]:ASP:OD1[3_455]	2.17	0.03

## 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	530/602 (88%)	482 (91%)	37 (7%)	11 (2%)	7 24
1	B	530/602 (88%)	482 (91%)	39 (7%)	9 (2%)	9 29
All	All	1060/1204 (88%)	964 (91%)	76 (7%)	20 (2%)	8 26

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	380	GLN
1	B	51	LYS
1	B	361	VAL
1	B	496	THR
1	B	506	GLU
1	A	496	THR
1	B	118	PHE
1	B	281	PRO
1	A	116	GLY
1	A	281	PRO
1	A	361	VAL
1	B	116	GLY
1	A	253	SER
1	A	488	THR
1	B	54	ASP
1	A	381	ARG
1	A	506	GLU
1	A	515	ARG
1	B	81	MET

### 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	456/521 (88%)	442 (97%)	14 (3%)	40 71
1	B	456/521 (88%)	445 (98%)	11 (2%)	49 77
All	All	912/1042 (88%)	887 (97%)	25 (3%)	43 74

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	48	SER
1	A	51	LYS
1	A	89	SER

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Mol	Chain	Res	Type
1	A	96	ASN
1	A	168	LEU
1	A	190	LYS
1	A	248	LYS
1	A	265	ARG
1	A	308	GLU
1	A	324	ASP
1	A	367	GLU
1	A	453	ARG
1	A	476	LYS
1	B	12	LYS
1	B	81	MET
1	B	166	MET
1	B	248	LYS
1	B	252	CYS
1	B	348	LYS
1	B	363	GLU
1	B	427	LYS
1	B	471	TRP
1	B	520	ARG
1	B	528	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	A	172	GLN
1	A	223	GLN
1	A	266	ASN
1	A	517	GLN
1	B	10	ASN
1	B	77	HIS
1	B	145	ASN
1	B	159	ASN
1	B	415	ASN
1	B	481	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 monosaccharides in this entry.

## 5.6 Ligand geometry [\(i\)](#)

1 ligand is 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	8U2	A	601	-	47,47,47	3.06	14 (29%)	53,67,67	4.57	32 (60%)

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	8U2	A	601	-	3/3/4/5	8/16/38/38	0/7/6/6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	8U2	NBA-NAZ	9.88	1.53	1.34
2	A	601	8U2	CAG-NAJ	9.57	1.44	1.32
2	A	601	8U2	CAW-NAZ	6.46	1.59	1.47
2	A	601	8U2	CBC-CAY	5.90	1.57	1.51
2	A	601	8U2	CAI-CAB	-5.45	1.37	1.44
2	A	601	8U2	CAH-CAM	-5.24	1.43	1.51
2	A	601	8U2	CBE-CBF	-4.73	1.41	1.51
2	A	601	8U2	CAA-CAB	-3.68	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	8U2	CAD-CAE	2.56	1.41	1.36
2	A	601	8U2	CAQ-CAO	-2.48	1.46	1.52
2	A	601	8U2	CAX-NAZ	2.41	1.38	1.35
2	A	601	8U2	CAP-CAO	2.30	1.58	1.52
2	A	601	8U2	OBN-CBI	2.30	1.41	1.36
2	A	601	8U2	CAN-CAO	-2.09	1.47	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	8U2	CAQ-CAO-CAP	15.97	131.28	113.27
2	A	601	8U2	CAM-CAN-CAO	-9.86	76.04	110.60
2	A	601	8U2	CAH-CAG-NAJ	-9.23	119.54	123.66
2	A	601	8U2	CAP-CAG-NAJ	7.35	127.87	116.34
2	A	601	8U2	CAF-CAE-CL1	-7.28	107.97	119.35
2	A	601	8U2	CAB-CAC-NAJ	-6.95	115.44	122.81
2	A	601	8U2	CAD-CAE-CL1	6.69	128.01	119.64
2	A	601	8U2	CAE-CAD-CAC	-6.34	114.15	119.50
2	A	601	8U2	CBF-CBE-NBL	-6.07	100.04	113.05
2	A	601	8U2	CAS-CAR-CAT	5.98	123.06	112.51
2	A	601	8U2	CAA-CAB-CAC	5.69	124.70	118.33
2	A	601	8U2	CBP-OBO-CBJ	-5.20	109.69	117.53
2	A	601	8U2	CAQ-CAR-CAS	5.15	119.36	109.65
2	A	601	8U2	CAA-CAB-CAI	-4.99	112.21	123.08
2	A	601	8U2	CBE-NBL-CBD	4.97	130.08	122.34
2	A	601	8U2	CAN-CAM-CAH	4.78	117.17	111.64
2	A	601	8U2	CAG-CAP-CAO	-4.63	102.38	112.18
2	A	601	8U2	CAD-CAC-NAJ	4.34	125.33	118.72
2	A	601	8U2	CAM-CAS-CAR	-4.26	95.65	110.60
2	A	601	8U2	CAW-NAZ-CAX	3.86	138.90	129.82
2	A	601	8U2	CAQ-CAO-CAN	3.70	116.64	109.65
2	A	601	8U2	OBO-CBJ-CBK	-3.45	118.18	124.12
2	A	601	8U2	OBO-CBJ-CBI	3.43	119.53	114.57
2	A	601	8U2	CAX-NAZ-NBA	-3.21	103.02	109.45
2	A	601	8U2	CAG-NAJ-CAC	3.13	121.54	117.67
2	A	601	8U2	CAS-CAM-CAN	3.09	113.25	109.52
2	A	601	8U2	CAH-CAI-NAL	-3.04	117.28	121.11
2	A	601	8U2	CAF-CAA-CAB	-2.73	117.34	121.13
2	A	601	8U2	CAQ-CAR-CAT	2.63	117.15	112.51
2	A	601	8U2	OBM-CBD-NBL	2.08	126.94	123.01
2	A	601	8U2	CBK-CBJ-CBI	2.07	122.28	120.06
2	A	601	8U2	NBB-NBA-NAZ	-2.02	105.79	107.31

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	8U2	CAR
2	A	601	8U2	CAO
2	A	601	8U2	CAM

All (8) torsion outliers are listed below:

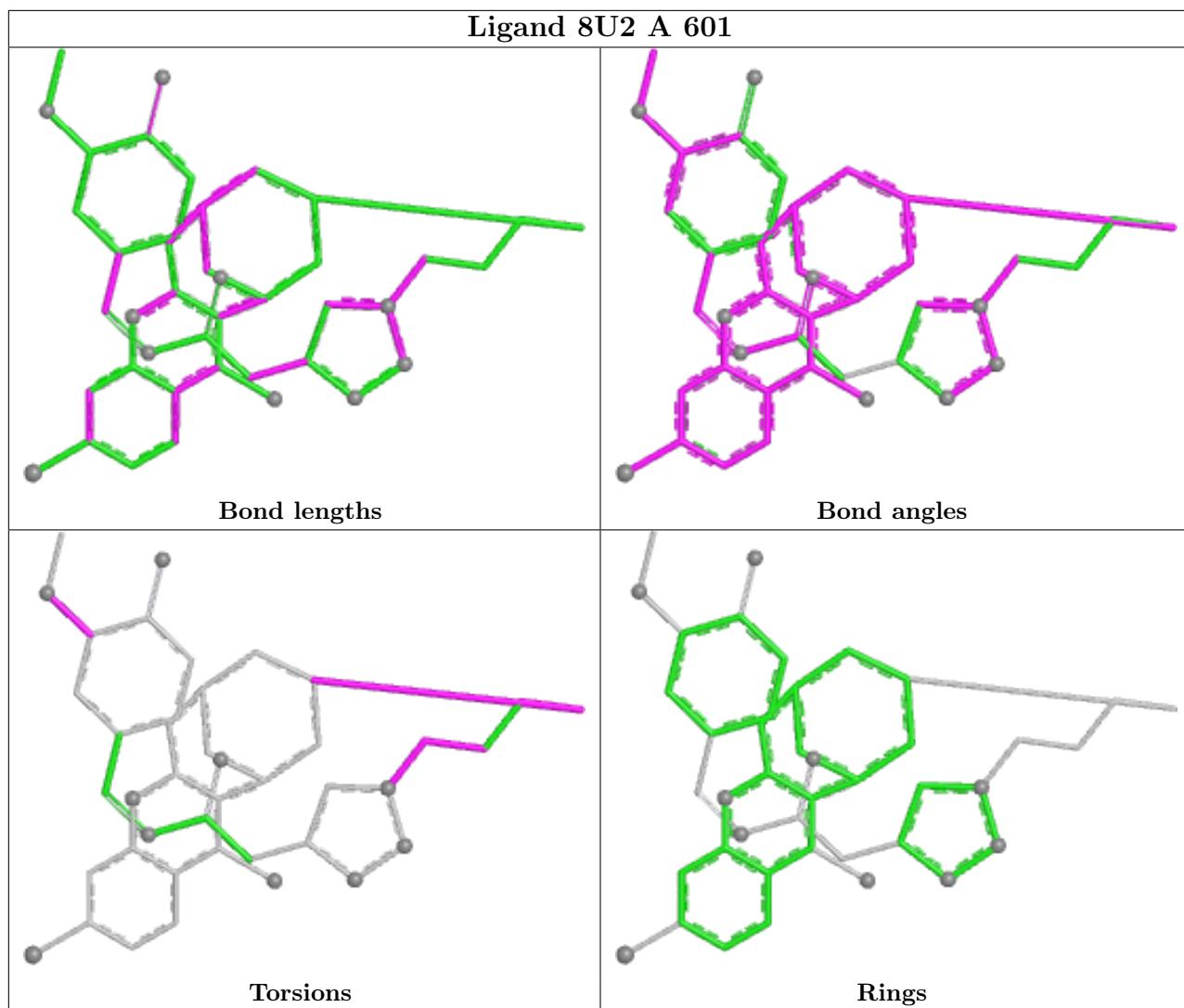
Mol	Chain	Res	Type	Atoms
2	A	601	8U2	CAV-CAW-NAZ-CAX
2	A	601	8U2	CAU-CAV-CAW-NAZ
2	A	601	8U2	CBK-CBJ-OBO-CBP
2	A	601	8U2	CAQ-CAR-CAT-CAU
2	A	601	8U2	CBI-CBJ-OBO-CBP
2	A	601	8U2	CAS-CAR-CAT-CAU
2	A	601	8U2	CAR-CAT-CAU-CAV
2	A	601	8U2	CAV-CAW-NAZ-NBA

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	8U2	5	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 [\(i\)](#)

### 6.1 Protein, DNA and RNA chains [\(i\)](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	527/602 (87%)	0.39	26 (4%) 29 29	51, 75, 103, 127	6 (1%)
1	B	527/602 (87%)	0.36	28 (5%) 26 25	38, 73, 102, 136	5 (0%)
All	All	1054/1204 (87%)	0.38	54 (5%) 28 27	38, 74, 103, 136	11 (1%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	481	ASN	4.8
1	B	53	SER	4.7
1	B	345	ILE	4.2
1	B	15	GLY	3.9
1	B	237	TYR	3.8
1	B	360	GLY	3.7
1	B	484	GLN	3.7
1	A	52	TRP	3.7
1	A	12	LYS	3.5
1	A	3	ASP	3.5
1	B	4	ILE	3.3
1	A	375[A]	ASP	3.3
1	B	529	VAL	3.3
1	B	100	PRO	3.2
1	B	22	GLY	3.2
1	B	366	LYS	3.1
1	B	378	ASP	3.1
1	B	485	ASN	3.0
1	A	53	SER	3.0
1	B	379	ASP	3.0
1	B	52	TRP	2.9
1	A	214[A]	HIS	2.9
1	A	344	ILE	2.8
1	B	17	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	453	ARG	2.8
1	B	3	ASP	2.8
1	A	376	TRP	2.7
1	A	366	LYS	2.7
1	A	35[A]	GLN	2.6
1	A	335	PRO	2.6
1	B	99	ILE	2.6
1	A	368	SER	2.6
1	A	529	VAL	2.5
1	A	50	THR	2.5
1	B	214[A]	HIS	2.5
1	A	7	ALA	2.4
1	B	215	SER	2.4
1	A	10	ASN	2.4
1	A	177	TRP	2.3
1	B	361	VAL	2.3
1	B	198	SER	2.3
1	B	13	VAL	2.2
1	A	13	VAL	2.2
1	A	483	THR	2.2
1	B	385	TYR	2.2
1	B	259	GLU	2.1
1	A	379	ASP	2.1
1	A	481	ASN	2.1
1	B	269	PRO	2.1
1	B	348	LYS	2.1
1	A	348	LYS	2.1
1	A	9	LYS	2.1
1	A	336	GLY	2.1
1	A	372[A]	HIS	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 [\(i\)](#)

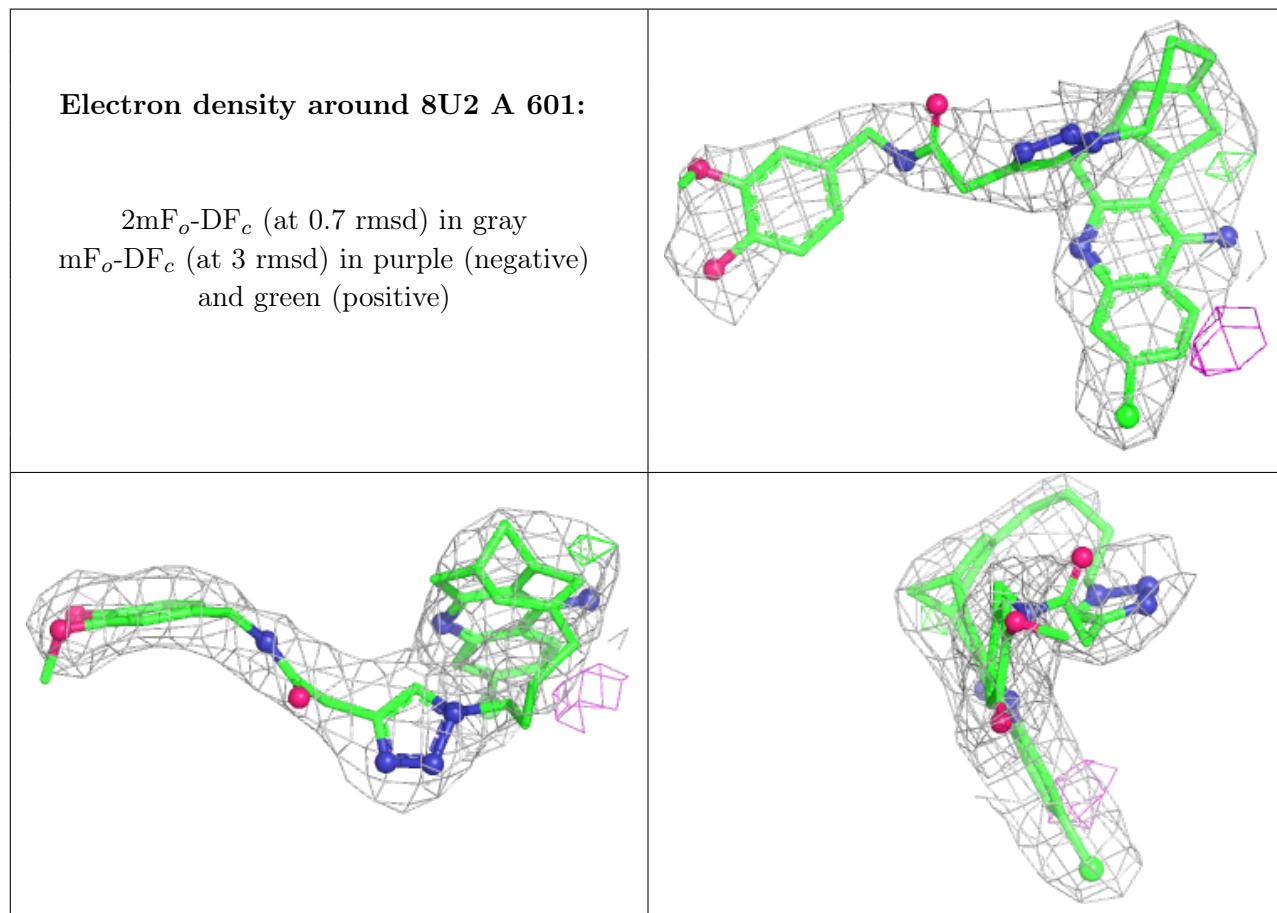
There are no monosaccharides in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	8U2	A	601	42/42	0.89	0.24	59,76,90,91	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.



## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.