



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:42 AM UTC

PDB ID : 7AIY / pdb_00007aiy
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

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

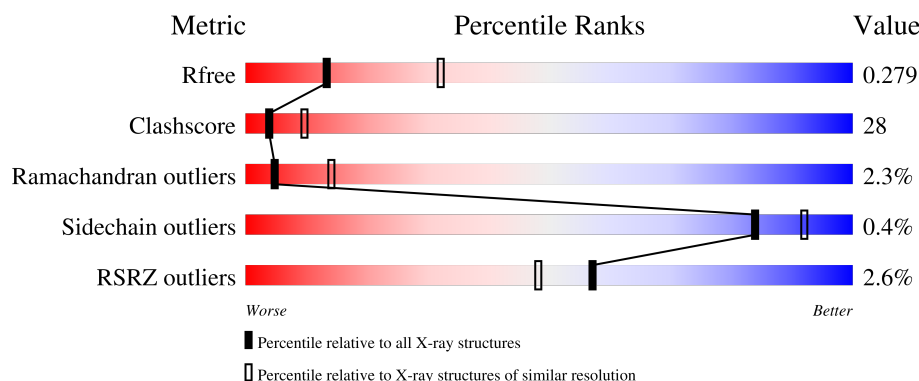
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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}	180053	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	602	
1	B	602	

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](#)

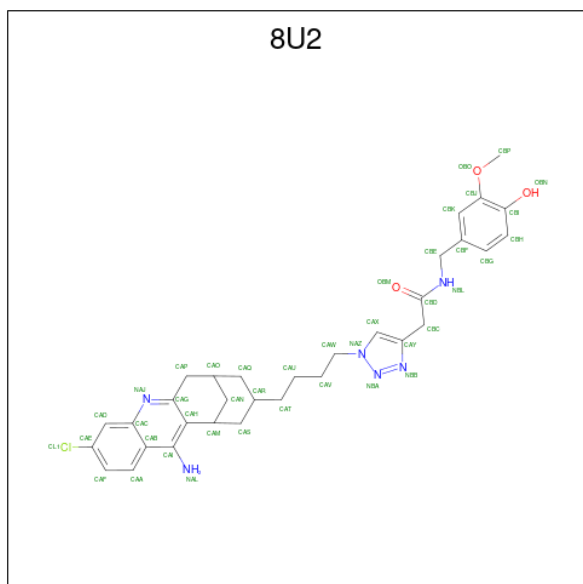
There are 2 unique types of molecules in this entry. The entry contains 8498 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	5	5	0
			4228	2725	714	774	15			
1	B	527	Total	C	N	O	S	5	5	0
			4228	2725	714	774	15			

- 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 (CCD ID: 8U2) (formula: C₃₂H₃₇ClN₆O₃) (labeled as "Ligand of Interest" by depositor).

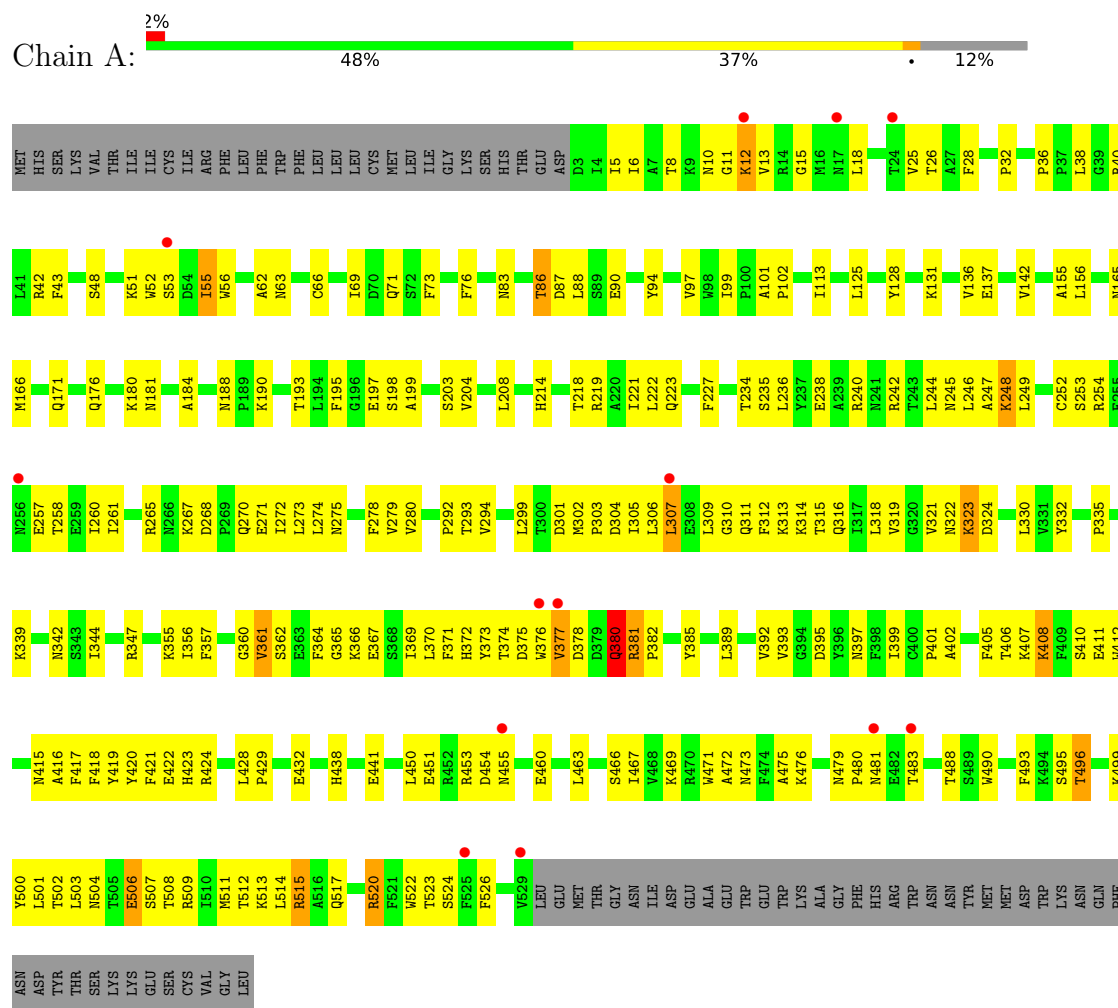


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			42	32	1	6	3		

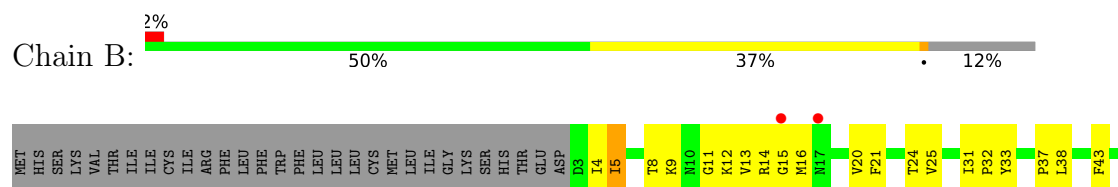
3 Residue-property plots

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



• Molecule 1: Cholinesterase



R520	F521	W522	T523	S524	F525	F526	F527	K528	V529	LEU	GLU	MET	THR	GLY	ASN	ILE	ASP	GLU	ALA	GLU	TRP	TRP	LYS	ALA	GLY	PHE	HIS	ARG	TRP	ASN	ASN	TYR	MET	MET	ASP	TRP	LYS	ASN	GLN	PHE	ASN	ASP	TYR	THR	SER	LYS	LYS	GLU	SER	CYS	VAL	GLY	LEU
L428	P429	W430	P431	E432	E441	F444	V445	P449	L450	D454	M455	Y456	T457	K458	I462	R465	K469	P480	M481	T483	T488	S489	W490	P491	V492	F493	K494	S495	T496	Y500	L501	T502	L503	M504	T505	E506	S507	T508	R509	I510	M511	T512	K513	L514	R515	A516	C519						
F350	Q351	E352	Q353	L354	K355	I356	F357	F358	P359	Q360	V361	F364	G365	K366	E367	S368	I369	L370	F371	H372	Y373	T374	D375	W376	V377	D378	D379	Q380	R381	P382	E383	N384	Y385	R386	E387	L388	L389	D395	I399	C400	L403	F409	N414	M415	A416	F417	F418	Y419	H423	R424	S425		
D268	F269	L273	E276	V279	V280	P281	V288	W289	F290	V294	D295	F298	L299	T300	D301	K302	P303	D304	I305	L306	L307	E308	L309	G310	Q311	F312	K313	K314	T315	Q316	I317	L318	V319	K323	D324	L330	V331	Y332	P335	Q336	F337	S338	K339	N342	T346	R347	K348	E349					
L49	T50	K51	W52	S53	D54	I55	W56	N57	A58	T59	N63	S64	G65	C66	Q67	N68	I69	F76	H77	G78	K81	P84	S89	L93	Y94	T99	P100	A101	P102	K103	P104	K105	I111	G116	G117	F118	Q119	T122	S123	K131	R135	V136	E137	N145	Y146	R147							
F153	L154	A155	L156	P163	G164	M165	M166	G167	F169	D170	L175	Q176	W177	V178	M181	F185	F195	G200	V204	L208	L209	R214	A220	I221	F227	E238	A239	R240	W241	R242	T243	K248	C252	S253	R254	E255	W256	E257	T258	E259	I260	L261											

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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) 81.0 (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 (Not available) , 0.279	Depositor DCC
R_{free} test set	1358 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	63.2	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8498	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 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	0.60	5/4357 (0.1%)	0.89	14/5918 (0.2%)
1	B	0.50	0/4357	0.86	8/5918 (0.1%)
All	All	0.55	5/8714 (0.1%)	0.88	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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	520	ARG	NE-CZ	-10.35	1.21	1.33
1	A	520	ARG	CZ-NH2	-8.64	1.22	1.33
1	A	520	ARG	CD-NE	-8.26	1.34	1.46
1	A	520	ARG	CZ-NH1	-8.25	1.21	1.32
1	A	36	PRO	C-N	-5.50	1.21	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	SER	N-CA-C	11.66	125.18	110.61
1	A	55	ILE	CG1-CB-CG2	-9.15	83.24	110.70
1	A	53	SER	N-CA-C	9.00	123.82	112.03
1	B	53	SER	CA-C-N	8.81	137.56	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	SER	C-N-CA	8.81	137.56	121.70
1	A	323	LYS	CD-CE-NZ	8.12	137.87	111.90
1	A	53	SER	CA-C-N	7.35	134.94	121.70
1	A	53	SER	C-N-CA	7.35	134.94	121.70
1	B	360	GLY	CA-C-N	6.98	134.27	121.70
1	B	360	GLY	C-N-CA	6.98	134.27	121.70
1	A	408	LYS	CB-CG-CD	-6.91	95.42	111.30
1	B	53	SER	CA-C-O	-6.58	114.36	121.20
1	A	380	GLN	CA-C-N	6.33	137.24	121.80
1	A	380	GLN	C-N-CA	6.33	137.24	121.80
1	A	12	LYS	CA-CB-CG	6.19	126.48	114.10
1	A	307	LEU	CB-CA-C	5.84	121.39	110.70
1	A	377	VAL	CA-C-N	5.44	131.49	121.70
1	A	377	VAL	C-N-CA	5.44	131.49	121.70
1	A	55	ILE	CA-CB-CG1	5.34	119.48	110.40
1	B	385	TYR	CA-CB-CG	-5.25	104.45	113.90
1	B	5	ILE	CA-CB-CG1	-5.19	101.58	110.40
1	A	248	LYS	CA-CB-CG	5.17	124.44	114.10

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	257	1
1	B	4228	0	4125	219	1
2	A	42	0	0	5	0
All	All	8498	0	8247	473	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 28.

All (473) 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:A:506:GLU:CD	1:A:507:SER:H	1.75	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: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:361:VAL:HG12	1:A:366:LYS:HZ2	1.37	0.86
1:B:16:MET:HE2	1:B:59:THR:OG1	1.75	0.86
1:B:16:MET:HE2	1:B:59:THR:CA	2.06	0.86
1:B:16:MET:HE2	1:B:59:THR:HA	1.57	0.85
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: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:B:294:VAL:HG21	1:B:302:MET:HE2	1.67	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
1:A:355:LYS:CE	1:A:366:LYS:HE2	2.15	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:323:LYS:NZ	1:A:420:TYR:CD2	2.56	0.74
1:B:16:MET:CE	1:B:59:THR:HA	2.17	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: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:422:GLU:CD	1:A:509:ARG:HH22	1.97	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:451:GLU:HG3	1:A:454:ASP:CG	2.15	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: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:479:ASN:OD1	1:A:481:ASN:CG	2.35	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:253:SER:C	1:A:254:ARG:HD3	2.19	0.67
1:A:62:ALA:O	1:A:86:THR:HG21	1.93	0.67
1:B:380:GLN:HG2	1:B:381:ARG:N	2.09	0.67
1:B:432:GLU:O	1:B:432:GLU:HG2	1.95	0.66
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:PRO:HD2	1:B:166:MET:HE3	1.76	0.65
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:323:LYS:HZ1	1:A:420:TYR:C	2.05	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: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:361:VAL:HG12	1:A:366:LYS:HZ1	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:A:378:ASP:H	1:A:380:GLN:CD	2.09	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:5:ILE:HD11	1:B:13:VAL:C	2.26	0.60
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:B:164:GLY:H	1:B:166:MET:HE1	1.66	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:B:16:MET:HE2	1:B:59:THR:CB	2.31	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:361:VAL:CG1	1:A:366:LYS:HZ2	2.13	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:21:PHE:C	1:B:135:ARG:HH12	2.10	0.58
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: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:A:323:LYS:NZ	1:A:420:TYR:C	2.63	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:165:ASN:HD22	1:B:295:ASP:CG	2.13	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:B:68:ASN:OD1	1:B:273:LEU:HB3	2.06	0.56
1:A:495:SER:O	1:A:496:THR:OG1	2.19	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:A:323:LYS:HE2	1:A:421:PHE:C	2.31	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ASN:O	1:A:246:LEU:C	2.49	0.56
1:B:238:GLU:O	1:B:242:ARG:HG3	2.05	0.56
1:B:111:ILE:HD11	1:B:178:VAL:HG21	1.87	0.56
1:B:528:LYS:HD2	1:B:528:LYS:C	2.31	0.56
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:A:411:GLU:OE1	1:A:495:SER:OG	2.13	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:43:PHE:O	1:B:166:MET:HE2	2.06	0.54
1:B:66:CYS:HB3	1:B:273:LEU:HD11	1.90	0.54
1:B:376:TRP:HB3	1:B:378:ASP:C	2.33	0.54
1:A:40:ARG:O	1:A:265:ARG:NH1	2.41	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:260:ILE:HG22	1:A:261:ILE:HG12	1.90	0.53
1:A:376:TRP:HB3	1:A:378:ASP:C	2.33	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:8:THR:OG1	1:B:11:GLY:O	2.22	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:381:ARG:HH12	1:B:387:GLU:CD	2.18	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:208:LEU:O	1:A:214[B]:HIS:NE2	2.41	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: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: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:B:78:GLY:HA2	1:B:81:MET:HE3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:HIS:NE2	2:A:601:8U2:NAL	2.59	0.50
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:370:LEU:O	1:A:371:PHE:C	2.55	0.49
1:A:307:LEU:C	1:A:408:LYS:CE	2.85	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: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:253:SER:C	1:B:254:ARG:HG2	2.38	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:12:LYS:HZ1	1:B:54:ASP:C	2.20	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:A:43:PHE:HA	1:A:166:MET:HE3	1.96	0.48
1:B:252:CYS:O	1:B:260:ILE:HG22	2.13	0.48
1:B:525:PHE:CD1	1:B:525:PHE:C	2.91	0.48
1:A:376:TRP:C	1:A:378:ASP:HA	2.38	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:B:12:LYS:HZ2	1:B:55:ILE:HB	1.78	0.48
1:A:69:ILE:HG23	1:A:83:ASN:CG	2.38	0.48
1:B:352:GLU:HA	1:B:355:LYS:HE3	1.94	0.48
1:A:364:PHE:O	1:A:365:GLY:C	2.57	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:B:373:TYR:OH	1:B:395:ASP:OD1	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:100:PRO:HD2	1:B:104:PRO:HG2	1.96	0.47
1:B:525:PHE:C	1:B:527:PRO:HD2	2.39	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:177:TRP:NE1	1:B:181:ASN:HD22	2.12	0.47
1:A:378:ASP:H	1:A:380:GLN:NE2	2.12	0.47
1:B:258:THR:O	1:B:261:ILE:HG13	2.15	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:377:VAL:C	1:A:380:GLN:HE22	2.23	0.47
1:A:101:ALA:HA	1:A:102:PRO:C	2.38	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:A:278:PHE:C	1:A:280:VAL:H	2.22	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: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:B:419:TYR:C	1:B:419:TYR:CD2	2.94	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:PRO:C	1:B:38:LEU:HD23	2.42	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:378:ASP:C	1:A:380:GLN:H	2.24	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:4:ILE:HD11	1:B:15:GLY:C	2.42	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
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:B:56:TRP:CD1	1:B:56:TRP:C	2.94	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: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: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:A:370:LEU:C	1:A:374:THR:HG23	2.41	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:245:ASN:O	1:A:248:LYS:CD	2.66	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:16:MET:HE2	1:B:59:THR:C	2.42	0.43
1:B:146:TYR:HB2	1:B:170:ASP:HB2	2.01	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:A:198:SER:OG	1:A:199:ALA:N	2.49	0.43
1:B:67:GLN:CD	1:B:84:PRO:HG3	2.44	0.43
1:B:335:PRO:HB2	1:B:349:GLU:HB3	2.01	0.43
1:A:410:SER:C	1:A:412:TRP:H	2.27	0.43
1:B:526:PHE:N	1:B:527:PRO:HD2	2.34	0.43
1:A:520:ARG:O	1:A:524:SER:OG	2.20	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: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:101:ALA:HA	1:B:102:PRO:C	2.44	0.42
1:B:368:SER:O	1:B:371:PHE:HB3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:146:TYR:HD1	1:B:147:ARG:O	2.02	0.42
1:B:400:CYS:HA	1:B:403:LEU:HD12	2.01	0.42
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: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:227:PHE:CD2	1:B:227:PHE:C	2.98	0.41
1:B:370:LEU:O	1:B:374:THR:HG22	2.19	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:376:TRP:C	1:B:378:ASP:HA	2.46	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: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:307:LEU:C	1:A:408:LYS:NZ	2.78	0.41
1:A:373:TYR:C	1:A:375[B]:ASP:H	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:303:PRO:O	1:B:304:ASP:C	2.64	0.41
1:B:308:GLU:O	1:B:308:GLU:HG2	2.19	0.41
1:B:364:PHE:O	1:B:365:GLY:C	2.63	0.41
1:A:13:VAL:HG23	1:A:52:TRP:HZ2	1.86	0.41
1:A:307:LEU:C	1:A:408:LYS:HE2	2.45	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
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:188:ASN:C	1:A:190:LYS:H	2.30	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:278:PHE:C	1:A:280:VAL:N	2.79	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

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	169/602 (28%)	147 (87%)	15 (9%)	7 (4%)	2	5
1	B	530/602 (88%)	482 (91%)	39 (7%)	9 (2%)	7	20
All	All	699/1204 (58%)	629 (90%)	54 (8%)	16 (2%)	5	14

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	361	VAL
1	B	116	GLY
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 ⓘ

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%)	454 (100%)	2 (0%)	84	92
1	B	456/521 (88%)	454 (100%)	2 (0%)	84	92
All	All	912/1042 (88%)	908 (100%)	4 (0%)	84	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	86	THR
1	B	81	MET
1	B	252	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	A	172	GLN
1	A	517	GLN
1	B	10	ASN
1	B	77	HIS
1	B	145	ASN
1	B	159	ASN
1	B	172	GLN
1	B	351	GLN
1	B	415	ASN
1	B	481	ASN
1	B	498	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 oligosaccharides 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	3.14	16 (34%)	60,67,67	4.16	33 (55%)

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	8/18/38/38	0/7/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	8U2	NAZ-NBA	11.64	1.53	1.34
2	A	601	8U2	CAG-NAJ	10.06	1.44	1.32
2	A	601	8U2	CAI-CAB	-5.53	1.37	1.44
2	A	601	8U2	CAH-CAM	-5.33	1.43	1.51
2	A	601	8U2	CBE-CBF	-4.64	1.41	1.51
2	A	601	8U2	CAW-NAZ	4.62	1.59	1.47
2	A	601	8U2	CAA-CAB	-3.78	1.34	1.42
2	A	601	8U2	NBB-NBA	3.69	1.38	1.32
2	A	601	8U2	CBC-CAY	3.41	1.57	1.50
2	A	601	8U2	CAD-CAE	2.74	1.41	1.36
2	A	601	8U2	CBC-CBD	2.68	1.55	1.51
2	A	601	8U2	CAY-NBB	-2.44	1.32	1.36
2	A	601	8U2	CAQ-CAO	-2.38	1.46	1.52
2	A	601	8U2	OBN-CBI	2.35	1.41	1.36
2	A	601	8U2	CAP-CAO	2.28	1.58	1.52
2	A	601	8U2	CAN-CAO	-2.00	1.47	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	8U2	CAM-CAN-CAO	-9.86	76.04	110.60
2	A	601	8U2	CAH-CAG-NAJ	-9.37	119.54	123.65
2	A	601	8U2	CAI-CAB-CAC	8.66	123.06	118.23
2	A	601	8U2	CAX-NAZ-NBA	-7.94	103.02	110.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	8U2	CAF-CAE-CL1	-7.72	107.97	119.36
2	A	601	8U2	CAP-CAG-NAJ	7.15	127.87	116.39
2	A	601	8U2	CAB-CAC-NAJ	-6.95	115.44	122.80
2	A	601	8U2	CAD-CAE-CL1	6.95	128.01	119.65
2	A	601	8U2	CAE-CAD-CAC	-6.45	114.15	119.47
2	A	601	8U2	CBF-CBE-NBL	-6.18	100.04	113.07
2	A	601	8U2	CAS-CAR-CAT	5.75	123.06	112.28
2	A	601	8U2	CAA-CAB-CAC	5.69	124.70	118.36
2	A	601	8U2	CAW-NAZ-CAX	5.39	138.90	128.83
2	A	601	8U2	CBP-OBO-CBJ	-5.34	109.69	117.51
2	A	601	8U2	CAA-CAB-CAI	-5.17	112.21	123.06
2	A	601	8U2	CAQ-CAR-CAS	5.09	119.36	109.69
2	A	601	8U2	CAG-CAP-CAO	-4.89	102.38	111.77
2	A	601	8U2	CBE-NBL-CBD	4.71	130.08	122.42
2	A	601	8U2	CAD-CAC-NAJ	4.47	125.33	118.78
2	A	601	8U2	CAN-CAM-CAH	4.37	117.17	111.52
2	A	601	8U2	CAM-CAS-CAR	-4.26	95.65	110.60
2	A	601	8U2	CAX-CAY-NBB	3.71	112.64	108.12
2	A	601	8U2	CAQ-CAO-CAN	3.65	116.64	109.69
2	A	601	8U2	OBO-CBJ-CBK	-3.42	118.18	124.08
2	A	601	8U2	OBO-CBJ-CBI	3.32	119.53	114.55
2	A	601	8U2	CAG-NAJ-CAC	3.26	121.54	117.67
2	A	601	8U2	CAY-CAX-NAZ	3.19	109.80	105.33
2	A	601	8U2	CAS-CAM-CAN	3.15	113.25	109.55
2	A	601	8U2	CAH-CAI-NAL	-3.04	117.28	121.11
2	A	601	8U2	CAF-CAA-CAB	-2.72	117.34	121.15
2	A	601	8U2	CAQ-CAR-CAT	2.59	117.15	112.28
2	A	601	8U2	CBK-CBJ-CBI	2.22	122.28	120.04
2	A	601	8U2	CBC-CBD-NBL	-2.04	113.58	116.25

All (3) chirality outliers are listed below:

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

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	8U2	CAU-CAV-CAW-NAZ
2	A	601	8U2	CBK-CBJ-OBO-CBP

Continued on next page...

Continued from previous page...

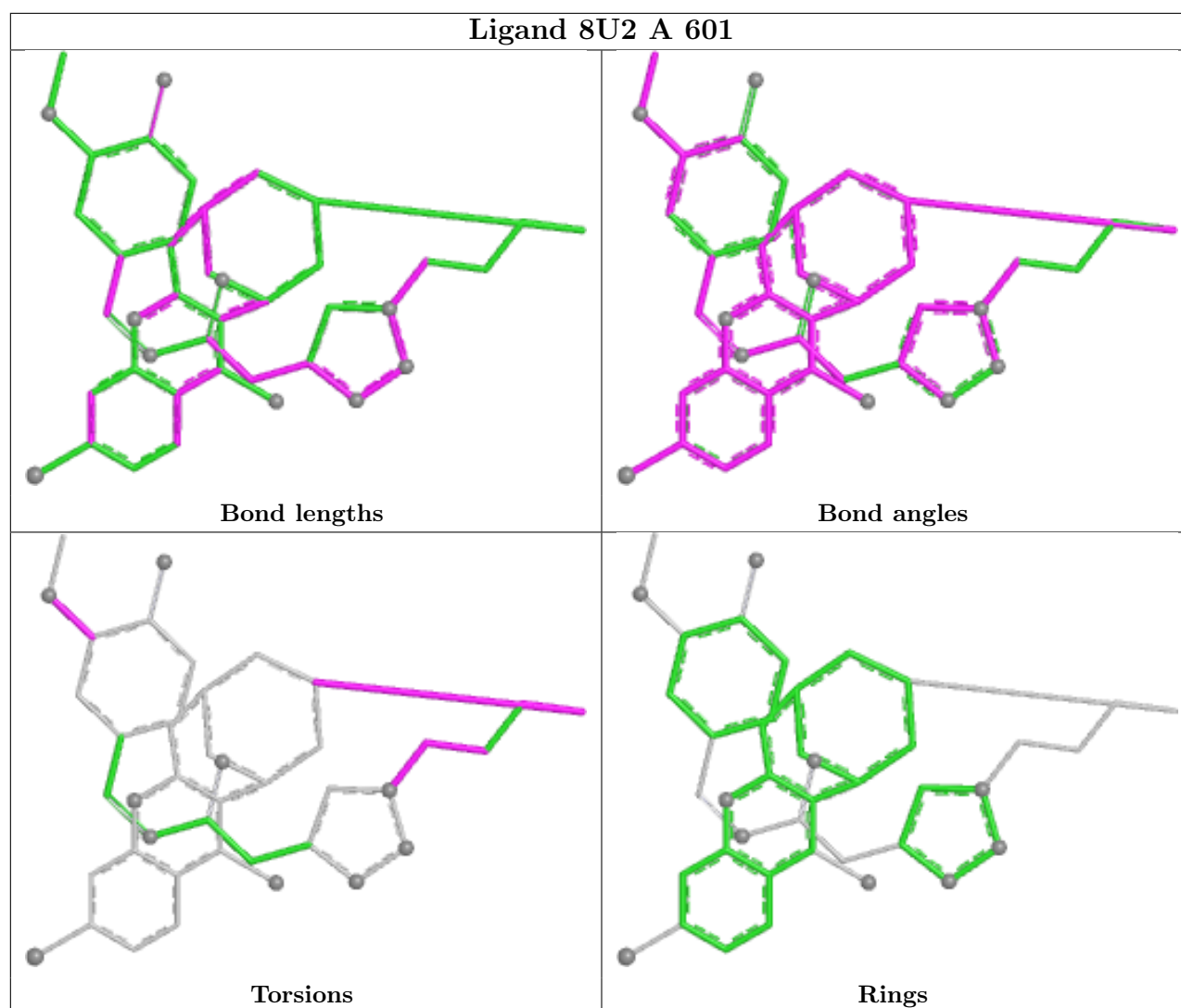
Mol	Chain	Res	Type	Atoms
2	A	601	8U2	CAQ-CAR-CAT-CAU
2	A	601	8U2	CBI-CBJ-OBO-CBP
2	A	601	8U2	CAS-CAR-CAT-CAU
2	A	601	8U2	CAR-CAT-CAU-CAV
2	A	601	8U2	CAV-CAW-NAZ-CAX
2	A	601	8U2	CAV-CAW-NAZ-NBA

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

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	527/602 (87%)	0.24	13 (2%)	58 49	38, 74, 102, 127	11 (2%)
1	B	527/602 (87%)	0.17	14 (2%)	56 47	34, 72, 102, 136	10 (1%)
All	All	1054/1204 (87%)	0.21	27 (2%)	57 48	34, 74, 102, 136	21 (1%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	481	ASN	5.9
1	A	525	PHE	3.9
1	A	481	ASN	3.8
1	A	529	VAL	3.7
1	B	529	VAL	3.6
1	A	307	LEU	3.3
1	B	15	GLY	3.3
1	B	377	VAL	3.2
1	A	12	LYS	3.1
1	B	483	THR	3.0
1	B	17	ASN	2.9
1	B	52	TRP	2.9
1	B	375[A]	ASP	2.7
1	B	53	SER	2.6
1	A	377	VAL	2.6
1	B	176[A]	GLN	2.5
1	A	53	SER	2.5
1	B	58	ALA	2.5
1	A	256	ASN	2.4
1	A	24	THR	2.3
1	A	376	TRP	2.3
1	B	360	GLY	2.3
1	A	455	ASN	2.2
1	A	17	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	483	THR	2.2
1	B	385	TYR	2.1
1	B	528	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

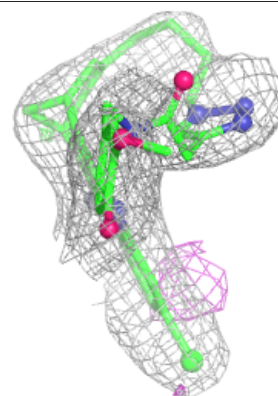
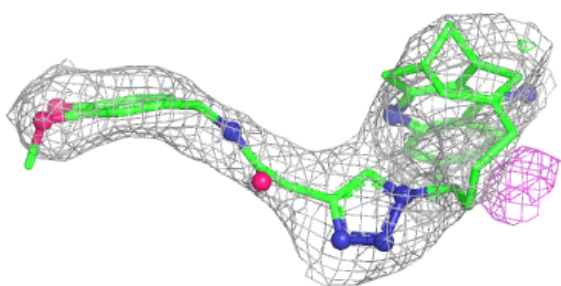
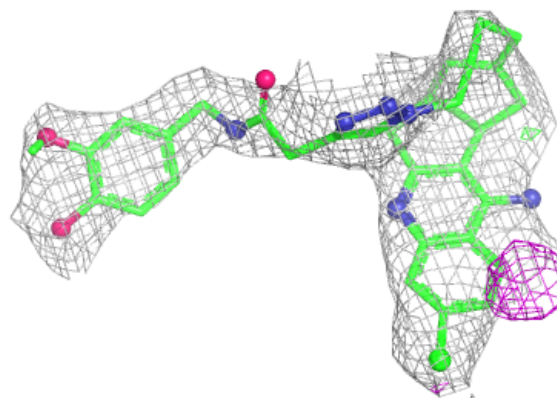
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	8U2	A	601	42/42	0.88	0.12	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.

Electron density around 8U2 A 601:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.