



Full wwPDB EM Validation Report ⓘ

May 25, 2025 – 12:33 AM JST

PDB ID : 9L4D / pdb_00009l4d
EMDB ID : EMD-62811
Title : ATR-ATRIP bound with RP-3500
Authors : Wang, G.
Deposited on : 2024-12-20
Resolution : 3.79 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

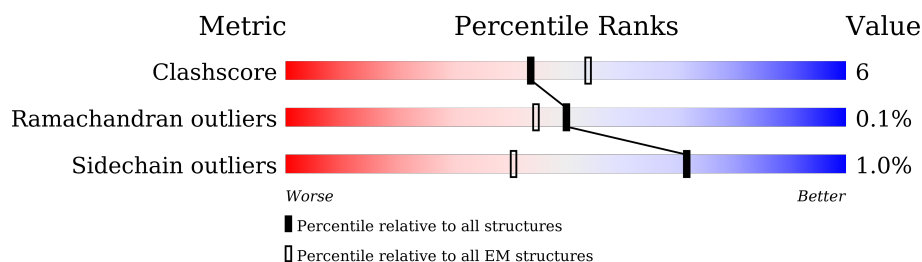
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.79 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	2637	
1	B	2637	
2	C	491	
2	D	491	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 67221 atoms, of which 29861 are hydrogens and 0 are deuteriums.

In the tables below, 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.

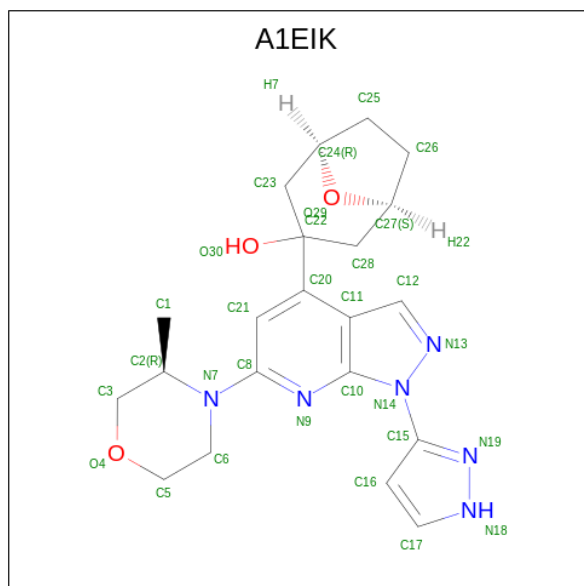
- Molecule 1 is a protein called Serine/threonine-protein kinase ATR.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2473	Total	C	H	N	O	S	0	0
			26772	9217	11475	2847	3181	52		
1	B	2497	Total	C	H	N	O	S	0	0
			31311	10642	14272	3025	3281	91		

- Molecule 2 is a protein called ATR-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	382	Total	C	H	N	O	S	0	0
			4498	1510	2026	462	485	15		
2	C	382	Total	C	H	N	O	S	0	0
			4579	1521	2088	461	485	24		

- Molecule 3 is RP-3500 (CCD ID: A1EIK) (formula: $C_{21}H_{26}N_6O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			30	21	6	3	
3	B	1	Total	C	N	O	0
			30	21	6	3	

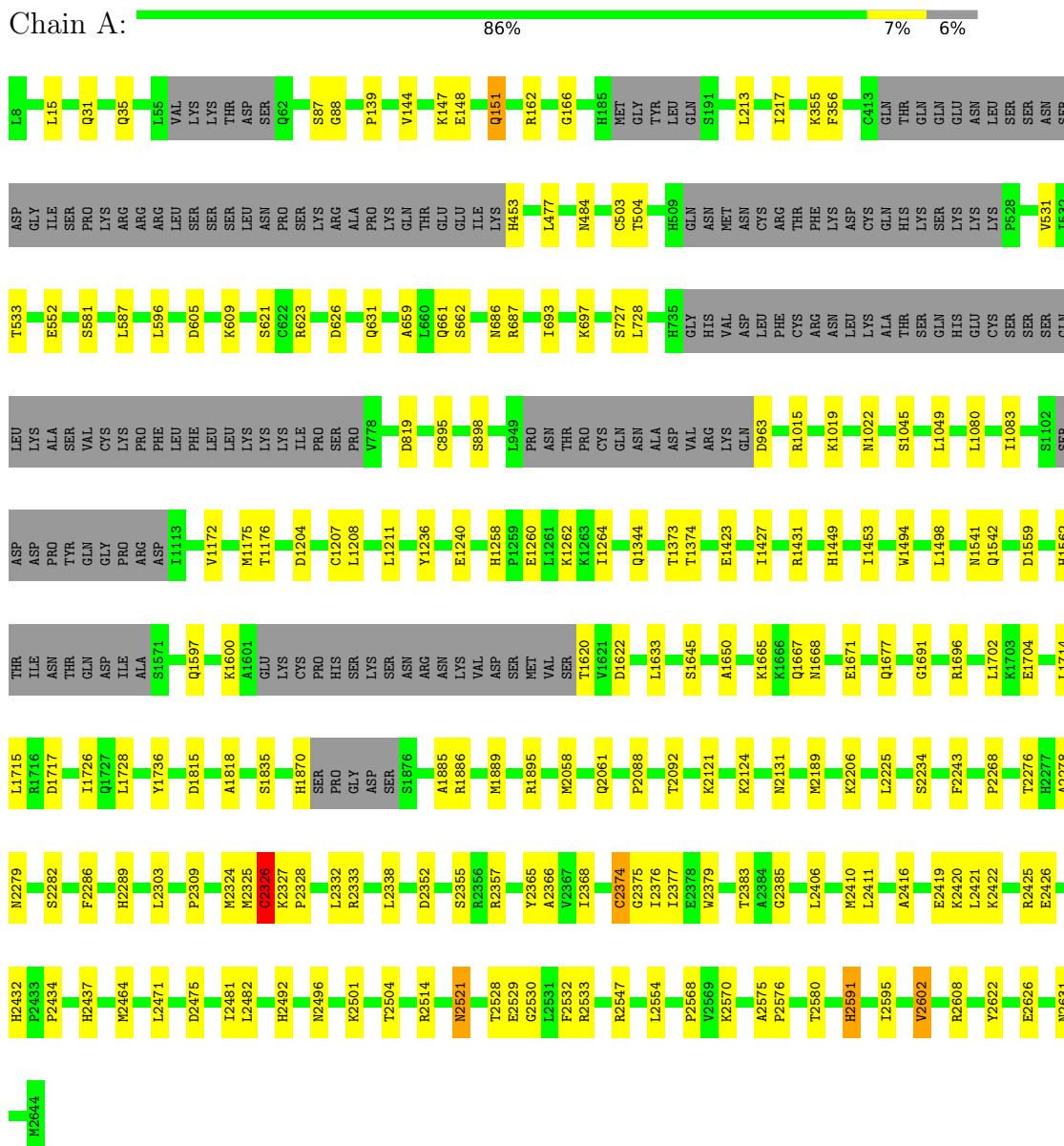
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total	Zn	0
			1	1	

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. 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. 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: Serine/threonine-protein kinase ATR



- Molecule 1: Serine/threonine-protein kinase ATR

81% 13% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77631	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

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: ZN, A1EIK

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	0.34	10/15382 (0.1%)	0.50	16/21057 (0.1%)
1	B	0.38	6/17289 (0.0%)	0.62	38/23571 (0.2%)
2	C	0.45	2/2513 (0.1%)	0.82	12/3426 (0.4%)
2	D	0.69	6/2493 (0.2%)	0.72	7/3401 (0.2%)
All	All	0.40	24/37677 (0.1%)	0.60	73/51455 (0.1%)

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	3
1	B	0	5
2	D	0	2
All	All	0	10

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	330	CYS	C-O	-23.55	0.93	1.24
2	D	330	CYS	C-N	-5.83	1.25	1.33
1	B	751	HIS	ND1-CE1	5.61	1.38	1.32
1	B	737	HIS	ND1-CE1	5.45	1.38	1.32
1	B	830	HIS	ND1-CE1	5.42	1.38	1.32
1	A	1870	HIS	ND1-CE1	5.37	1.38	1.32
1	A	2289	HIS	ND1-CE1	5.28	1.37	1.32
1	A	2437	HIS	ND1-CE1	5.27	1.37	1.32
2	D	535	GLN	CD-OE1	5.22	1.33	1.23
1	A	661	GLN	CD-OE1	5.18	1.33	1.23
2	D	584	GLN	CD-OE1	5.16	1.33	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	GLN	CD-OE1	5.15	1.33	1.23
2	D	588	GLN	CD-OE1	5.15	1.33	1.23
1	A	2631	ASN	CG-OD1	5.14	1.33	1.23
1	B	1542	GLN	CD-OE1	5.12	1.33	1.23
2	D	563	GLN	CD-OE1	5.11	1.33	1.23
1	A	2131	ASN	CG-OD1	5.09	1.33	1.23
1	A	1022	ASN	CG-OD1	5.08	1.33	1.23
1	A	2591	HIS	ND1-CE1	5.08	1.37	1.32
1	A	2521	ASN	CG-OD1	5.08	1.33	1.23
2	C	432	GLN	CD-OE1	5.08	1.33	1.23
1	B	2521	ASN	CG-OD1	5.05	1.33	1.23
1	B	2123	ASN	CG-OD1	5.02	1.33	1.23
2	C	584	GLN	CD-OE1	5.01	1.33	1.23

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	682	CYS	N-CA-CB	14.97	132.13	110.12
2	D	330	CYS	N-CA-CB	14.64	134.69	110.39
1	B	1188	PHE	CB-CA-C	-13.90	89.17	110.02
1	B	1189	PRO	N-CA-C	-13.87	94.82	113.40
1	B	1767	THR	CA-CB-OG1	-11.30	92.64	109.60
2	C	681	GLN	N-CA-C	-10.70	88.02	110.80
1	B	1191	LEU	CA-C-N	-10.08	106.58	120.38
1	B	1191	LEU	C-N-CA	-10.08	106.58	120.38
2	C	331	HIS	N-CA-C	-10.07	100.31	111.28
1	B	1355	GLY	N-CA-C	-9.76	101.02	112.73
1	B	1767	THR	CA-C-O	-9.71	110.26	120.55
2	D	330	CYS	O-C-N	-8.83	110.59	122.43
2	C	331	HIS	CA-C-O	-8.53	111.50	120.55
1	B	2326	CYS	N-CA-CB	8.31	122.23	109.85
2	D	334	SER	N-CA-C	-8.30	102.24	111.28
1	B	2324	MET	O-C-N	-8.22	113.39	123.33
2	C	320	PRO	N-CA-CB	-7.80	96.17	103.19
2	C	330	CYS	CB-CA-C	-7.70	96.38	110.63
1	B	1185	LYS	N-CA-C	-7.21	103.11	110.97
1	A	2326	CYS	N-CA-CB	7.15	120.63	109.83
1	B	1190	GLU	CA-C-N	7.11	129.80	120.28
1	B	1190	GLU	C-N-CA	7.11	129.80	120.28
1	B	2327	LYS	CB-CA-C	6.95	117.05	110.17
1	B	830	HIS	CB-CG-CD2	-6.70	122.50	131.20
1	B	1189	PRO	N-CA-CB	6.68	110.92	103.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2307	GLN	CB-CA-C	6.68	121.28	109.72
1	A	2591	HIS	CB-CG-CD2	-6.66	122.54	131.20
1	B	751	HIS	CB-CG-CD2	-6.66	122.55	131.20
1	A	1208	LEU	CA-C-O	-6.65	110.81	120.13
1	A	2437	HIS	CB-CG-CD2	-6.59	122.64	131.20
1	A	2289	HIS	CB-CG-CD2	-6.58	122.64	131.20
2	C	682	CYS	N-CA-C	-6.57	104.12	111.28
1	B	737	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	A	1870	HIS	CB-CG-CD2	-6.53	122.71	131.20
1	A	2432	HIS	CB-CG-CD2	-6.51	122.74	131.20
2	D	330	CYS	N-CA-C	-6.49	104.63	112.54
1	B	2306	LEU	N-CA-C	-6.42	104.28	111.28
1	B	1191	LEU	CA-C-O	-6.38	113.79	120.55
1	B	1191	LEU	N-CA-CB	6.33	119.43	110.12
1	B	1188	PHE	N-CA-C	6.15	120.32	108.45
2	C	680	CYS	CA-CB-SG	6.12	128.48	114.40
1	B	1357	CYS	CB-CA-C	-6.03	100.78	110.79
1	B	1173	LYS	N-CA-C	-6.00	104.81	111.36
2	C	319	GLN	N-CA-C	-5.95	100.23	109.87
1	B	2375	GLY	CA-C-O	-5.90	115.68	121.76
1	B	1589	THR	N-CA-C	-5.85	104.81	111.07
1	B	830	HIS	CB-CG-ND1	5.78	131.37	122.70
1	A	1870	HIS	CB-CG-ND1	5.78	131.37	122.70
1	B	751	HIS	CB-CG-ND1	5.70	131.25	122.70
1	A	2324	MET	O-C-N	-5.70	116.66	123.27
1	A	2591	HIS	CB-CG-ND1	5.64	131.16	122.70
1	B	737	HIS	CB-CG-ND1	5.62	131.13	122.70
1	A	2437	HIS	CB-CG-ND1	5.62	131.13	122.70
2	D	332	LEU	N-CA-CB	5.62	118.37	110.12
1	A	2289	HIS	CB-CG-ND1	5.55	131.02	122.70
1	A	2432	HIS	CB-CG-ND1	5.53	131.00	122.70
2	D	330	CYS	CB-CA-C	-5.51	98.80	110.31
1	B	1354	CYS	CB-CA-C	5.38	120.05	109.72
1	B	1045	SER	CA-C-O	-5.38	115.86	121.99
1	B	2335	ASP	CA-C-N	5.38	127.93	120.29
1	B	2335	ASP	C-N-CA	5.38	127.93	120.29
2	C	681	GLN	N-CA-CB	5.29	119.42	110.49
2	C	682	CYS	CA-CB-SG	5.22	126.41	114.40
1	B	2325	MET	N-CA-C	5.21	117.40	108.90
1	B	1197	ASP	N-CA-C	-5.20	105.04	111.33
2	C	680	CYS	CA-C-O	-5.14	114.29	120.10
1	A	1208	LEU	CA-C-N	5.14	125.68	119.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1208	LEU	C-N-CA	5.14	125.68	119.98
1	B	2481	ILE	CA-C-O	-5.12	115.72	121.36
1	B	979	ALA	CA-C-O	-5.12	115.12	120.55
1	A	504	THR	N-CA-C	-5.07	105.94	111.82
1	B	504	THR	N-CA-C	-5.06	105.76	111.28
2	D	331	HIS	N-CA-C	-5.04	100.06	110.80

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2333	ARG	Sidechain
1	A	2475	ASP	Mainchain
1	A	2547	ARG	Sidechain
1	B	1194	ARG	Sidechain
1	B	1767	THR	Mainchain
1	B	2324	MET	Mainchain
1	B	2333	ARG	Sidechain
1	B	2363	ARG	Sidechain
2	D	305	SER	Mainchain
2	D	328	SER	Mainchain

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	15297	11475	11498	103	0
1	B	17039	14272	14390	220	0
2	C	2491	2088	2096	56	0
2	D	2472	2026	2034	55	0
3	A	30	0	0	1	0
3	B	30	0	0	0	0
4	C	1	0	0	0	0
All	All	37360	29861	30018	424	0

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 6.

All (424) 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)
2:D:330:CYS:O	2:D:331:HIS:C	2.08	0.91
2:D:330:CYS:O	2:D:330:CYS:SG	2.35	0.84
1:B:2514:ARG:HG3	1:B:2519:MET:HE1	1.62	0.82
1:A:2366:ALA:HB1	1:A:2368:ILE:HD11	1.62	0.81
2:C:680:CYS:C	2:C:682:CYS:H	1.88	0.81
2:C:680:CYS:C	2:C:682:CYS:N	2.49	0.71
2:D:752:MET:HE2	2:D:777:CYS:H	1.57	0.70
2:D:330:CYS:HB2	2:D:333:LEU:CB	2.24	0.67
1:B:2585:ASN:HB3	1:B:2588:ALA:HB2	1.76	0.66
1:B:1191:LEU:HA	1:B:1194:ARG:HE	1.62	0.64
1:B:279:HIS:HB3	1:B:283:MET:HE3	1.79	0.64
1:B:23:PRO:HA	1:B:26:TYR:HB3	1.79	0.64
2:D:330:CYS:O	2:D:332:LEU:N	2.31	0.64
1:A:2481:ILE:HD12	1:A:2514:ARG:HD3	1.80	0.64
1:B:724:LEU:HA	1:B:747:ALA:HA	1.81	0.63
1:B:901:ALA:HB1	2:D:746:HIS:HA	1.81	0.63
1:B:1149:LYS:O	1:B:1153:ASN:ND2	2.33	0.62
1:B:2303:LEU:HD12	1:B:2325:MET:HE2	1.81	0.62
2:C:319:GLN:O	2:C:320:PRO:C	2.42	0.59
1:B:890:LEU:HD23	1:B:893:LEU:HD12	1.83	0.59
2:D:752:MET:HE1	2:D:773:LEU:HA	1.83	0.59
1:B:2303:LEU:HD21	1:B:2311:LYS:HD2	1.84	0.58
2:D:330:CYS:C	2:D:332:LEU:N	2.56	0.58
1:B:763:CYS:O	1:B:767:LEU:N	2.27	0.57
2:C:378:ALA:HB1	2:C:422:LEU:HA	1.86	0.57
1:B:2332:LEU:HD22	1:B:2375:GLY:HA3	1.87	0.57
2:D:331:HIS:HB2	2:C:334:SER:CB	2.34	0.57
2:D:330:CYS:CB	2:D:333:LEU:CB	2.83	0.56
1:B:1366:PRO:O	1:B:2356:ARG:NH2	2.36	0.56
1:B:890:LEU:HD11	1:B:932:PRO:CB	2.37	0.55
2:D:310:SER:C	2:D:312:LEU:H	2.14	0.55
2:C:550:SER:HG	2:C:593:CYS:HG	1.54	0.54
1:B:1656:MET:HE3	1:B:2441:LEU:HD22	1.89	0.54
2:D:330:CYS:SG	2:D:333:LEU:CB	2.96	0.54
1:B:2332:LEU:HD23	1:B:2367:VAL:HG12	1.90	0.53
1:B:2511:VAL:HG12	1:B:2636:MET:HE3	1.91	0.53
1:B:2072:PHE:O	1:B:2075:SER:OG	2.24	0.53
2:D:330:CYS:O	2:D:333:LEU:N	2.41	0.53
2:D:330:CYS:SG	2:D:334:SER:N	2.82	0.53
1:A:2276:THR:C	1:A:2278:ALA:H	2.17	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:330:CYS:O	2:C:331:HIS:C	2.52	0.53
1:B:890:LEU:HD23	1:B:893:LEU:CD1	2.39	0.52
1:B:2551:MET:HE2	1:B:2592:VAL:HG13	1.91	0.52
2:C:736:LEU:HA	2:C:739:MET:HE2	1.90	0.52
1:A:1344:GLN:HB3	1:A:1835:SER:HA	1.90	0.52
1:B:1518:MET:HE2	1:B:1525:THR:HA	1.92	0.52
2:C:371:SER:O	2:C:375:LEU:N	2.41	0.52
1:A:1677:GLN:OE1	1:A:1696:ARG:NH2	2.41	0.52
1:B:1886:ARG:HA	1:B:1889:MET:HE3	1.91	0.52
1:A:2189:MET:HE3	1:A:2580:THR:HA	1.90	0.51
2:D:378:ALA:HB1	2:D:422:LEU:HA	1.93	0.51
1:A:1204:ASP:OD2	1:A:1207:CYS:N	2.39	0.51
1:A:2464:MET:HE3	1:A:2492:HIS:HB2	1.93	0.51
1:B:656:TYR:O	1:B:660:LEU:N	2.43	0.51
1:A:963:ASP:N	1:A:963:ASP:OD1	2.43	0.50
2:D:717:VAL:O	2:D:721:ARG:HG3	2.11	0.50
2:C:495:LEU:O	2:C:498:SER:OG	2.25	0.50
2:C:468:VAL:O	2:C:472:GLU:HG2	2.12	0.50
1:A:1373:THR:OG1	1:A:1374:THR:N	2.45	0.50
1:B:2466:MET:HE2	1:B:2540:MET:HG2	1.92	0.50
1:A:2234:SER:O	1:A:2234:SER:OG	2.30	0.50
1:B:2307:GLN:HG2	1:B:2328:PRO:HD2	1.94	0.50
1:A:2327:LYS:HB3	1:A:2332:LEU:HD11	1.93	0.49
2:D:330:CYS:C	2:C:330:CYS:SG	2.94	0.49
1:A:1886:ARG:HA	1:A:1889:MET:HE2	1.94	0.49
1:B:2332:LEU:O	1:B:2333:ARG:C	2.55	0.49
1:B:2466:MET:HE2	1:B:2540:MET:CG	2.42	0.49
1:B:1152:LEU:HG	1:B:1191:LEU:HD22	1.94	0.49
2:D:331:HIS:CB	2:C:334:SER:CB	2.89	0.49
1:A:2575:ALA:HB3	1:A:2576:PRO:HD3	1.94	0.49
2:D:388:LEU:O	2:D:392:ASN:N	2.45	0.49
1:A:87:SER:OG	1:A:88:GLY:N	2.45	0.48
2:C:680:CYS:CB	2:C:682:CYS:H	2.24	0.48
1:B:787:HIS:HA	1:B:830:HIS:CE1	2.47	0.48
2:D:328:SER:O	2:D:329:LEU:CB	2.60	0.48
2:C:718:ARG:HE	2:C:721:ARG:HD3	1.78	0.48
1:A:2591:HIS:O	1:A:2595:ILE:HG12	2.13	0.48
1:B:276:LEU:O	1:B:280:LEU:HG	2.13	0.48
1:A:2416:ALA:HB3	1:A:2419:GLU:HG3	1.95	0.48
1:B:70:ASP:HA	1:B:73:GLN:NE2	2.29	0.48
1:A:2501:LYS:O	1:A:2504:THR:OG1	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1309:GLU:HG3	1:B:1313:LYS:HZ2	1.79	0.48
2:C:330:CYS:O	2:C:330:CYS:SG	2.61	0.48
1:B:203:GLU:O	1:B:244:ILE:HD11	2.14	0.48
1:B:726:SER:HA	1:B:745:LEU:HD11	1.95	0.48
1:A:1494:TRP:O	1:A:1498:LEU:HG	2.14	0.48
1:A:2338:LEU:HD11	1:A:2471:LEU:HD13	1.96	0.48
1:B:91:GLU:HG2	1:B:92:ALA:N	2.29	0.48
2:D:476:VAL:HB	2:D:563:GLN:NE2	2.29	0.48
2:C:718:ARG:HA	2:C:721:ARG:HD3	1.95	0.48
1:A:2352:ASP:HB3	1:A:2355:SER:HB3	1.95	0.47
1:B:1581:VAL:HA	1:B:1584:MET:HG2	1.96	0.47
2:D:318:LYS:HD3	2:D:319:GLN:O	2.13	0.47
2:D:754:GLY:O	2:D:758:LEU:HD23	2.14	0.47
1:B:720:GLY:HA3	1:B:749:SER:HA	1.97	0.47
1:B:2457:TYR:O	1:B:2461:THR:HG22	2.14	0.47
2:C:469:CYS:SG	2:C:470:ILE:N	2.87	0.47
1:B:2303:LEU:HD21	1:B:2311:LYS:CD	2.45	0.47
1:B:813:MET:HE1	1:B:868:THR:HB	1.96	0.47
1:A:2568:PRO:C	1:A:2570:LYS:H	2.22	0.47
1:B:554:VAL:C	1:B:556:LYS:H	2.22	0.47
2:C:687:VAL:HG22	2:C:730:LEU:HD13	1.96	0.47
1:B:1212:LEU:HD22	1:B:1248:PHE:HB3	1.97	0.47
1:B:1993:GLY:O	1:B:1996:MET:HG2	2.14	0.47
1:B:2305:SER:HB2	1:B:2309:PRO:HD3	1.97	0.47
1:B:2511:VAL:H	1:B:2636:MET:CE	2.27	0.47
2:C:320:PRO:CB	2:C:325:SER:O	2.62	0.47
1:A:626:ASP:N	1:A:626:ASP:OD1	2.46	0.47
1:A:1895:ARG:HH12	1:A:2357:ARG:NH2	2.13	0.47
1:B:281:VAL:HG22	1:B:333:VAL:HG12	1.96	0.47
2:D:600:LEU:HD21	2:D:651:GLN:HB3	1.97	0.47
2:C:648:LEU:HD23	2:C:648:LEU:H	1.79	0.47
1:B:1675:PHE:HA	1:B:1678:LYS:HD3	1.97	0.47
1:B:213:LEU:HB3	1:B:251:PHE:CZ	2.50	0.46
1:B:1297:VAL:HG22	1:B:1300:ARG:HH21	1.79	0.46
1:B:832:LEU:HD12	1:B:879:ALA:HB3	1.97	0.46
2:D:556:LEU:O	2:D:560:VAL:HG23	2.15	0.46
1:B:251:PHE:O	1:B:255:LEU:HG	2.15	0.46
1:B:304:PRO:HB2	1:B:306:GLU:HG3	1.98	0.46
1:B:760:ALA:O	1:B:762:VAL:HG22	2.16	0.46
1:B:813:MET:HE3	1:B:869:LEU:HD22	1.96	0.46
1:B:1856:MET:HE1	1:B:1899:PRO:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2174:GLN:HA	1:B:2266:MET:HE1	1.97	0.46
1:B:2380:VAL:HG23	1:B:2383:THR:HG21	1.97	0.46
1:B:53:VAL:HG11	1:B:115:SER:C	2.40	0.46
1:B:1212:LEU:O	1:B:1216:ILE:HG12	2.15	0.46
1:B:1163:GLY:HA3	1:B:1202:CYS:C	2.41	0.46
1:A:605:ASP:O	1:A:609:LYS:HG2	2.14	0.46
1:A:2608:ARG:HG3	1:B:2052:MET:HG3	1.98	0.46
1:B:279:HIS:O	1:B:283:MET:HG2	2.16	0.46
1:B:352:TYR:HA	1:B:356:PHE:HD2	1.80	0.46
1:B:1354:CYS:HA	1:B:1357:CYS:CB	2.45	0.46
1:B:1355:GLY:HA2	1:B:1831:ILE:HD11	1.97	0.46
1:B:1234:PHE:CE2	1:B:1264:ILE:HG21	2.50	0.46
2:C:632:LEU:CB	2:C:682:CYS:HB3	2.46	0.46
1:B:203:GLU:O	1:B:207:VAL:HG23	2.15	0.46
1:B:382:VAL:O	1:B:386:GLU:HG2	2.16	0.46
1:B:890:LEU:HA	1:B:893:LEU:HD12	1.96	0.46
1:B:2182:VAL:HG12	1:B:2194:CYS:HB2	1.98	0.46
1:B:2385:GLY:C	1:B:2388:PRO:HD2	2.41	0.46
1:B:296:SER:O	1:B:300:LYS:HD3	2.16	0.46
1:B:688:VAL:H	1:B:762:VAL:HG12	1.81	0.46
1:B:1798:THR:HG23	1:B:1803:ARG:NH2	2.30	0.46
1:B:2334:LYS:HB2	1:B:2563:VAL:HG21	1.98	0.46
1:B:217:ILE:HA	1:B:220:VAL:HG22	1.97	0.45
1:B:1924:TRP:HB3	1:B:1947:ALA:HB2	1.97	0.45
1:B:2154:ASP:N	1:B:2154:ASP:OD1	2.49	0.45
1:A:1691:GLY:HA3	1:A:2530:GLY:HA2	1.97	0.45
1:A:2225:LEU:HG	1:A:2243:PHE:CE2	2.52	0.45
1:A:2268:PRO:HA	1:A:2286:PHE:HD1	1.81	0.45
1:B:1166:HIS:O	1:B:1170:VAL:HG12	2.17	0.45
1:B:1403:ALA:C	1:B:1406:ALA:H	2.24	0.45
1:B:2332:LEU:CD2	1:B:2375:GLY:HA3	2.46	0.45
2:D:600:LEU:HD13	2:D:647:ALA:HB1	1.97	0.45
2:D:725:LEU:O	2:D:728:HIS:ND1	2.49	0.45
1:A:659:ALA:O	1:A:662:SER:OG	2.28	0.45
1:A:2279:ASN:HB3	1:A:2282:SER:OG	2.16	0.45
1:A:1702:LEU:HD22	1:A:1728:LEU:HD12	1.98	0.45
1:A:2379:TRP:HA	3:A:2701:A1EIK:C3	2.47	0.45
1:A:31:GLN:O	1:A:35:GLN:N	2.50	0.45
1:A:1559:ASP:HB3	1:A:1562:HIS:NE2	2.32	0.45
1:A:1895:ARG:HH22	1:A:2357:ARG:CZ	2.29	0.45
1:B:73:GLN:HB3	1:B:77:LYS:NZ	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ARG:HD2	1:B:223:ARG:N	2.32	0.45
1:B:2434:PRO:HB2	1:B:2521:ASN:OD1	2.16	0.45
2:C:662:LEU:HD23	2:C:663:LEU:HD22	1.99	0.45
1:A:1645:SER:OG	1:A:1650:ALA:O	2.34	0.45
1:B:2280:HIS:C	1:B:2282:SER:H	2.23	0.45
1:A:2385:GLY:N	1:A:2482:LEU:HD23	2.32	0.45
1:B:1188:PHE:CB	1:B:1192:CYS:H	2.30	0.45
1:B:1339:LEU:HD22	1:B:1354:CYS:SG	2.57	0.45
1:B:2136:TYR:O	1:B:2139:LEU:HB3	2.17	0.45
2:C:482:LEU:O	2:C:486:VAL:HG22	2.17	0.45
1:A:213:LEU:O	1:A:217:ILE:N	2.50	0.45
1:B:327:VAL:HA	1:B:330:GLU:HG2	1.99	0.45
1:B:2022:MET:HE3	1:B:2022:MET:HB3	1.76	0.45
1:B:2325:MET:HE3	1:B:2379:TRP:CZ3	2.52	0.45
2:D:304:ARG:O	2:D:305:SER:C	2.60	0.45
2:D:741:CYS:O	2:D:745:LEU:N	2.50	0.45
1:B:1309:GLU:HG3	1:B:1313:LYS:NZ	2.32	0.44
1:B:1639:ASP:OD1	1:B:1639:ASP:N	2.51	0.44
1:A:727:SER:OG	1:A:728:LEU:N	2.50	0.44
1:A:1633:LEU:HD23	1:A:1633:LEU:HA	1.89	0.44
1:B:124:CYS:O	1:B:125:GLU:C	2.60	0.44
2:C:539:LEU:HD23	2:C:542:LEU:HD21	2.00	0.44
1:A:1597:GLN:O	1:A:1600:LYS:HG3	2.17	0.44
1:A:2121:LYS:HA	1:A:2124:LYS:HE2	1.99	0.44
1:B:53:VAL:HG23	1:B:55:LEU:H	1.82	0.44
1:B:1542:GLN:HG3	1:B:1546:GLN:NE2	2.32	0.44
2:C:478:ALA:HA	2:C:481:ILE:HD12	1.99	0.44
1:B:340:ASP:N	1:B:340:ASP:OD1	2.51	0.44
1:B:2248:LYS:HE3	1:B:2248:LYS:HB3	1.85	0.44
1:B:2548:GLU:HB2	1:B:2549:PRO:HD3	2.00	0.44
1:A:1260:GLU:O	1:A:1264:ILE:HG12	2.18	0.44
1:A:1620:THR:OG1	1:A:1622:ASP:OD1	2.32	0.44
1:A:1815:ASP:CB	1:A:1818:ALA:HB3	2.48	0.44
1:B:106:ARG:HH21	1:B:109:ARG:HD3	1.82	0.44
1:B:1190:GLU:O	1:B:1193:CYS:CB	2.66	0.44
1:B:2119:LEU:O	1:B:2123:ASN:OD1	2.35	0.44
2:C:556:LEU:O	2:C:560:VAL:HG22	2.17	0.44
1:A:552:GLU:O	1:A:623:ARG:NH1	2.50	0.44
1:A:1015:ARG:O	1:A:1019:LYS:HG2	2.17	0.44
1:A:1175:MET:HE3	1:A:1211:LEU:HD12	2.00	0.44
1:B:134:PHE:HD2	1:B:141:ILE:HG21	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2585:ASN:HD21	1:B:2587:LYS:HG2	1.83	0.44
2:C:418:HIS:C	2:C:421:PRO:HD2	2.42	0.44
1:B:1191:LEU:HA	1:B:1194:ARG:NE	2.31	0.44
2:D:332:LEU:O	2:D:335:SER:O	2.36	0.44
2:D:486:VAL:O	2:D:574:ASN:ND2	2.51	0.44
1:B:171:TRP:HB2	1:B:172:PRO:HD3	1.99	0.44
1:B:1307:LEU:O	1:B:1311:LEU:HG	2.18	0.44
1:B:1337:THR:O	1:B:1341:LYS:HG2	2.18	0.44
1:B:2076:LEU:HD23	1:B:2076:LEU:HA	1.79	0.44
2:D:314:ASN:O	2:D:318:LYS:HB2	2.18	0.44
2:C:420:LEU:HD11	2:C:538:LEU:HD22	1.99	0.44
2:C:630:CYS:SG	2:C:630:CYS:O	2.75	0.44
1:B:2389:ILE:HG23	1:B:2439:TRP:CD1	2.53	0.43
1:A:1045:SER:O	1:A:1049:LEU:N	2.40	0.43
1:A:2434:PRO:HB2	1:A:2521:ASN:OD1	2.18	0.43
1:B:817:ASP:OD2	1:B:820:VAL:HG23	2.18	0.43
1:B:2035:TRP:CZ2	1:B:2037:ASP:HB2	2.53	0.43
1:B:2467:VAL:O	1:B:2471:LEU:HB2	2.18	0.43
1:A:355:LYS:HG3	1:A:356:PHE:N	2.33	0.43
1:B:760:ALA:C	1:B:762:VAL:H	2.25	0.43
1:B:1150:MET:SD	1:B:1150:MET:N	2.91	0.43
1:B:1668:ASN:O	1:B:1671:GLU:HG2	2.18	0.43
2:C:725:LEU:HD12	2:C:725:LEU:HA	1.79	0.43
2:D:331:HIS:CG	2:D:332:LEU:N	2.83	0.43
1:A:2528:THR:O	1:A:2532:PHE:HB3	2.19	0.43
1:A:2568:PRO:O	1:A:2570:LYS:HD3	2.19	0.43
1:B:373:ARG:O	1:B:377:LYS:HG2	2.18	0.43
1:B:1190:GLU:H	1:B:1194:ARG:HH21	1.67	0.43
1:B:1757:ASN:HA	1:B:1760:HIS:HB3	2.01	0.43
2:D:753:PRO:O	2:D:757:MET:HG2	2.19	0.43
1:A:2088:PRO:O	1:A:2092:THR:OG1	2.33	0.43
1:B:153:PHE:O	1:B:157:VAL:HG22	2.19	0.43
1:B:2340:GLU:O	1:B:2343:SER:OG	2.30	0.43
2:D:652:TRP:O	2:D:656:GLU:HG2	2.19	0.43
2:C:381:LEU:O	2:C:384:THR:OG1	2.35	0.43
2:C:472:GLU:OE1	2:C:560:VAL:HG11	2.17	0.43
1:A:693:ILE:O	1:A:697:LYS:HG2	2.18	0.43
1:B:2005:LEU:HD12	1:B:2005:LEU:HA	1.84	0.43
1:A:2326:CYS:HA	1:A:2376:ILE:HA	2.01	0.43
1:B:704:LYS:NZ	1:B:774:ILE:HG23	2.33	0.43
1:B:2058:MET:HA	1:B:2061:GLN:CD	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2539:THR:O	1:B:2543:MET:HG2	2.19	0.43
2:C:629:GLY:O	2:C:682:CYS:SG	2.77	0.43
1:A:453:HIS:CE1	1:A:533:THR:HG23	2.53	0.43
1:A:1431:ARG:HD2	1:A:1431:ARG:HA	1.74	0.43
1:A:1449:HIS:O	1:A:1453:ILE:HG12	2.19	0.43
1:B:285:THR:OG1	1:B:286:ASP:N	2.52	0.43
1:B:1595:LYS:O	1:B:1599:LEU:HG	2.19	0.43
2:C:418:HIS:O	2:C:421:PRO:HD2	2.19	0.43
1:A:2622:TYR:O	1:A:2626:GLU:HG2	2.19	0.43
1:B:735:HIS:CE1	1:B:738:VAL:HA	2.54	0.43
1:B:1635:LEU:HD23	1:B:1635:LEU:HA	1.88	0.43
1:B:2512:PRO:HB2	1:B:2513:PHE:CD1	2.53	0.43
1:B:12:ILE:N	1:B:13:PRO:HD2	2.34	0.42
1:B:135:LYS:HA	1:B:142:PHE:HB2	2.01	0.42
1:B:261:LEU:HD12	1:B:262:PRO:HD2	2.01	0.42
1:B:1318:LEU:O	1:B:1322:ALA:N	2.50	0.42
1:B:2498:LEU:HD23	1:B:2498:LEU:HA	1.86	0.42
1:B:2516:THR:H	1:B:2519:MET:HE3	1.84	0.42
2:C:489:SER:OG	2:C:490:GLY:N	2.52	0.42
1:B:1862:HIS:ND1	1:B:1881:LEU:HD21	2.34	0.42
2:D:601:PRO:O	2:D:604:LEU:HG	2.19	0.42
1:A:162:ARG:O	1:A:166:GLY:N	2.52	0.42
1:B:901:ALA:N	2:D:781:THR:O	2.50	0.42
1:B:1098:ALA:HB1	1:B:1111:ARG:CB	2.50	0.42
1:B:1865:LYS:HE3	1:B:1877:GLN:HE22	1.84	0.42
1:B:1869:GLN:HG2	1:B:1877:GLN:HB3	2.01	0.42
1:A:144:VAL:O	1:A:148:GLU:HG3	2.20	0.42
1:A:2374:CYS:SG	1:A:2375:GLY:N	2.90	0.42
1:B:760:ALA:O	1:B:762:VAL:N	2.52	0.42
1:B:1767:THR:O	1:B:1767:THR:HG22	2.19	0.42
1:B:2238:SER:O	1:B:2242:HIS:ND1	2.52	0.42
2:D:716:THR:O	2:D:720:LEU:HG	2.19	0.42
2:C:377:GLU:O	2:C:381:LEU:HD23	2.19	0.42
1:A:1175:MET:HE2	1:A:1175:MET:HB2	1.95	0.42
1:A:2411:LEU:HD12	1:A:2420:LYS:HG2	2.01	0.42
1:B:1239:ILE:HA	1:B:1242:ARG:NH2	2.35	0.42
1:B:1800:TRP:CE3	1:B:1853:ARG:HD3	2.54	0.42
1:B:2063:ASP:OD1	1:B:2063:ASP:N	2.52	0.42
1:B:2157:PHE:CZ	1:B:2193:ARG:HD2	2.54	0.42
1:A:1240:GLU:N	1:A:1240:GLU:OE1	2.52	0.42
1:B:1784:TRP:HA	1:B:1787:VAL:HB	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2182:VAL:HA	1:B:2185:SER:OG	2.20	0.42
1:A:1258:HIS:O	1:A:1262:LYS:N	2.53	0.42
1:B:147:LYS:HD2	1:B:147:LYS:HA	1.73	0.42
1:B:317:TYR:O	1:B:321:LEU:HD23	2.19	0.42
1:B:2529:GLU:HG3	1:B:2533:ARG:HH21	1.84	0.42
2:C:428:GLY:O	2:C:432:GLN:HG3	2.19	0.42
1:A:1885:ALA:O	1:A:1889:MET:HG3	2.19	0.42
1:A:2554:LEU:HD23	1:A:2554:LEU:HA	1.91	0.42
1:B:554:VAL:C	1:B:556:LYS:N	2.77	0.42
1:B:1722:TYR:HB3	1:B:1739:VAL:HG23	2.01	0.42
2:D:653:LEU:HD11	2:D:716:THR:HA	2.01	0.42
1:A:1541:ASN:OD1	1:A:1542:GLN:N	2.53	0.42
1:B:101:ASN:HB3	1:B:178:PHE:O	2.19	0.42
1:B:714:LEU:HA	1:B:717:THR:HG22	2.02	0.42
1:B:1263:LYS:O	1:B:1267:VAL:HG13	2.19	0.42
1:B:1562:HIS:CE1	1:B:1563:THR:HG23	2.55	0.42
1:B:1570:ALA:HA	1:B:1573:LEU:HB3	2.01	0.42
1:B:2497:CYS:SG	1:B:2502:GLY:N	2.93	0.42
2:D:651:GLN:HA	2:D:654:GLN:CD	2.45	0.42
2:C:727:LEU:HD22	2:C:737:PHE:HZ	1.84	0.42
1:A:686:ASN:OD1	1:A:687:ARG:N	2.52	0.42
1:A:1080:LEU:O	1:A:1083:ILE:HG22	2.19	0.42
1:A:2276:THR:HB	1:A:2279:ASN:H	1.85	0.42
1:B:89:SER:O	1:B:93:LYS:N	2.42	0.42
1:B:230:TRP:O	1:B:234:CYS:HB2	2.20	0.42
1:B:703:VAL:HA	1:B:706:GLU:HG3	2.02	0.42
1:B:849:ARG:O	1:B:852:GLU:HG3	2.19	0.42
1:B:1658:PHE:O	1:B:1662:ILE:HG22	2.19	0.42
1:A:1696:ARG:HH12	1:A:1704:GLU:HB3	1.85	0.41
1:B:26:TYR:HE2	1:B:85:ASN:HB2	1.84	0.41
1:B:2529:GLU:HG3	1:B:2533:ARG:NH2	2.34	0.41
2:D:699:LEU:HA	2:D:702:ARG:HH21	1.85	0.41
2:C:389:VAL:HG13	2:C:415:GLY:HA3	2.01	0.41
1:B:2213:GLY:O	1:B:2217:ARG:HD3	2.19	0.41
1:B:2580:THR:HG22	1:B:2582:GLU:HB2	2.02	0.41
1:A:139:PRO:O	2:C:668:VAL:HA	2.20	0.41
1:B:352:TYR:HA	1:B:356:PHE:CD2	2.55	0.41
1:B:2019:ASN:HA	1:B:2022:MET:HB2	2.02	0.41
1:B:2259:LEU:HD12	1:B:2290:TRP:HB3	2.02	0.41
2:C:585:CYS:O	2:C:589:VAL:HG23	2.20	0.41
1:A:895:CYS:O	1:A:898:SER:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LYS:O	1:B:36:ILE:HG12	2.20	0.41
1:B:142:PHE:CZ	1:B:219:ILE:HG23	2.56	0.41
1:B:1288:SER:HB3	1:B:1307:LEU:HD12	2.02	0.41
1:B:1297:VAL:O	1:B:1301:ILE:HG12	2.20	0.41
1:B:1332:ILE:HG23	1:B:1361:LEU:HD21	2.03	0.41
1:B:1948:GLY:HA2	1:B:1955:LEU:HD22	2.02	0.41
1:B:2184:LYS:NZ	1:B:2219:THR:OG1	2.45	0.41
2:C:611:SER:O	2:C:665:LYS:NZ	2.54	0.41
1:A:1236:TYR:O	1:A:1240:GLU:HB2	2.20	0.41
1:B:12:ILE:O	1:B:16:ARG:HG2	2.20	0.41
1:B:256:PHE:HD1	1:B:301:THR:HG22	1.85	0.41
1:A:581:SER:OG	1:A:587:LEU:HD11	2.21	0.41
1:A:1172:VAL:O	1:A:1176:THR:HG23	2.21	0.41
1:A:2422:LYS:O	1:A:2426:GLU:HG2	2.20	0.41
1:B:1242:ARG:C	1:B:1244:ALA:H	2.28	0.41
1:B:1559:ASP:HB3	1:B:1562:HIS:ND1	2.36	0.41
1:B:1599:LEU:HD22	1:B:1623:TYR:CD1	2.55	0.41
1:B:2385:GLY:HA2	1:B:2482:LEU:HB3	2.02	0.41
1:A:1423:GLU:O	1:A:1427:ILE:HG12	2.20	0.41
1:A:1665:LYS:O	1:A:1667:GLN:HG2	2.20	0.41
1:B:1210:SER:O	1:B:1213:SER:OG	2.25	0.41
2:D:620:ALA:HB3	2:D:621:PRO:HD3	2.03	0.41
1:B:210:LEU:HD13	1:B:247:LEU:HB2	2.02	0.41
1:B:222:PHE:HB3	2:D:665:LYS:HD3	2.01	0.41
1:B:364:ALA:HB1	2:C:381:LEU:HD22	2.03	0.41
1:A:453:HIS:NE2	1:A:531:VAL:HG13	2.36	0.41
1:B:366:GLN:OE1	2:C:381:LEU:HD21	2.21	0.41
1:B:795:PHE:HD1	1:B:802:VAL:HG13	1.85	0.41
1:B:1481:SER:O	1:B:1483:LEU:N	2.54	0.41
1:B:1533:LEU:HD21	1:B:1632:PHE:HE2	1.85	0.41
1:B:1537:LEU:HD11	1:B:1632:PHE:CD2	2.56	0.41
1:B:2421:LEU:HD22	1:B:2631:ASN:OD1	2.21	0.41
2:D:373:SER:C	2:D:375:LEU:H	2.28	0.41
2:D:471:LEU:O	2:D:475:SER:N	2.53	0.41
2:D:564:CYS:HA	2:D:567:VAL:HG22	2.02	0.41
2:D:663:LEU:HD23	2:D:666:LEU:HD12	2.03	0.41
2:D:666:LEU:HD23	2:D:666:LEU:HA	1.96	0.41
2:D:721:ARG:HB3	2:D:769:GLU:OE1	2.21	0.41
2:C:427:ILE:HG22	2:C:541:MET:HG3	2.03	0.41
2:C:430:HIS:HA	2:C:433:ALA:HB3	2.02	0.41
2:C:693:MET:HA	2:C:696:ARG:HH11	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:LEU:HD22	1:A:621:SER:HB3	2.03	0.41
1:A:1714:LEU:HD23	1:A:1715:LEU:N	2.36	0.41
1:B:51:VAL:HG13	1:B:52:ALA:H	1.86	0.41
1:B:1191:LEU:CA	1:B:1194:ARG:HE	2.29	0.41
1:B:1315:GLN:O	1:B:1319:ILE:HG12	2.20	0.41
1:B:1702:LEU:O	1:B:1706:ILE:HG13	2.21	0.41
2:C:546:LEU:HD22	2:C:568:LEU:HD11	2.03	0.41
2:C:680:CYS:O	2:C:681:GLN:CB	2.69	0.41
1:A:477:LEU:HA	1:A:484:ASN:ND2	2.36	0.40
1:A:631:GLN:CD	1:A:631:GLN:H	2.29	0.40
1:A:2406:LEU:O	1:A:2410:MET:N	2.53	0.40
1:A:2421:LEU:HD11	1:A:2425:ARG:NH1	2.36	0.40
1:A:2422:LYS:HE3	1:A:2422:LYS:HB3	1.85	0.40
1:B:807:GLY:O	1:B:849:ARG:NH2	2.54	0.40
1:B:840:GLY:O	1:B:844:GLU:HG2	2.21	0.40
1:B:1559:ASP:H	1:B:1562:HIS:CE1	2.39	0.40
1:B:1912:LYS:HD2	1:B:1912:LYS:HA	1.91	0.40
2:D:728:HIS:O	2:D:732:GLN:OE1	2.39	0.40
2:C:710:THR:HG23	2:C:713:GLN:H	1.86	0.40
1:A:819:ASP:N	1:A:819:ASP:OD1	2.54	0.40
1:A:1726:ILE:HD11	1:A:1736:TYR:HA	2.04	0.40
1:A:2529:GLU:CD	1:A:2533:ARG:HE	2.29	0.40
1:B:320:MET:O	1:B:323:GLU:HG3	2.20	0.40
1:B:843:LYS:O	1:B:847:VAL:HG23	2.21	0.40
1:B:855:THR:O	1:B:858:GLN:HG3	2.20	0.40
1:B:2464:MET:HG2	1:B:2492:HIS:CD2	2.57	0.40
2:C:698:TRP:HA	2:C:701:VAL:HG12	2.03	0.40
1:A:147:LYS:O	1:A:151:GLN:OE1	2.38	0.40
1:A:2058:MET:HA	1:A:2061:GLN:CD	2.47	0.40
1:B:1212:LEU:HD13	1:B:1248:PHE:HD2	1.86	0.40
1:B:1221:PRO:O	1:B:1225:ILE:HG12	2.22	0.40
1:B:1325:SER:HA	1:B:2271:PRO:HA	2.04	0.40
1:B:1951:ARG:NH2	1:B:1983:CYS:SG	2.88	0.40
1:B:2058:MET:HA	1:B:2061:GLN:OE1	2.21	0.40
1:B:2221:LYS:HD3	1:B:2221:LYS:HA	1.89	0.40
2:C:610:LEU:HA	2:C:613:LEU:HD12	2.01	0.40
1:A:1668:ASN:HB3	1:A:1671:GLU:CD	2.46	0.40
1:A:1714:LEU:HD22	1:A:1717:ASP:HB2	2.03	0.40
1:A:2276:THR:HB	1:A:2279:ASN:HB2	2.03	0.40
1:A:2303:LEU:HD12	1:A:2309:PRO:HB2	2.02	0.40
1:A:2365:TYR:CD2	1:A:2377:ILE:HG23	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2410:MET:HE3	1:A:2410:MET:HB3	1.91	0.40
1:B:2042:LEU:HD11	1:B:2046:TYR:CZ	2.57	0.40
1:B:2269:THR:O	1:B:2283:HIS:NE2	2.51	0.40
1:B:2633:LEU:HD23	1:B:2633:LEU:HA	1.91	0.40
2:D:594:LEU:O	2:D:634:LEU:HD13	2.21	0.40
2:D:642:ARG:HB3	2:D:645:ARG:HH21	1.86	0.40
2:C:596:PRO:HA	2:C:638:TYR:CD2	2.57	0.40
2:C:709:ARG:HD3	2:C:709:ARG:H	1.86	0.40
1:A:2206:LYS:HA	1:A:2206:LYS:HD3	1.90	0.40
1:B:305:PHE:HD1	1:B:356:PHE:CE2	2.39	0.40
1:B:2086:SER:OG	1:B:2087:MET:N	2.55	0.40
2:D:416:ALA:HB3	2:D:492:VAL:HG21	2.03	0.40
2:D:429:LEU:HD12	2:D:429:LEU:HA	1.93	0.40
2:D:708:PRO:HG2	2:D:714:ARG:HG2	2.02	0.40
2:C:646:VAL:O	2:C:646:VAL:HG13	2.22	0.40

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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	2451/2637 (93%)	2313 (94%)	136 (6%)	2 (0%)	48	79
1	B	2471/2637 (94%)	2327 (94%)	142 (6%)	2 (0%)	48	79
2	C	370/491 (75%)	341 (92%)	27 (7%)	2 (0%)	25	58
2	D	372/491 (76%)	336 (90%)	35 (9%)	1 (0%)	37	69
All	All	5664/6256 (90%)	5317 (94%)	340 (6%)	7 (0%)	50	79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	557	LEU
2	D	329	LEU
2	C	318	LYS
1	A	2328	PRO
2	C	629	GLY
1	A	2602	VAL
1	B	904	SER

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 PDB entries followed by that with respect to all EM entries.

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	1021/2358 (43%)	1013 (99%)	8 (1%)	79	84
1	B	1387/2358 (59%)	1376 (99%)	11 (1%)	79	84
2	C	207/417 (50%)	201 (97%)	6 (3%)	37	58
2	D	194/417 (46%)	190 (98%)	4 (2%)	48	66
All	All	2809/5550 (51%)	2780 (99%)	29 (1%)	71	80

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	503	CYS
1	A	2325	MET
1	A	2326	CYS
1	A	2374	CYS
1	A	2383	THR
1	A	2496	ASN
1	A	2602	VAL
1	B	250	SER
1	B	1191	LEU
1	B	1712	LEU
1	B	2123	ASN
1	B	2305	SER
1	B	2326	CYS
1	B	2327	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2329	LYS
1	B	2377	ILE
1	B	2380	VAL
1	B	2567	LYS
2	D	330	CYS
2	D	334	SER
2	D	335	SER
2	D	535	GLN
2	C	330	CYS
2	C	432	GLN
2	C	584	GLN
2	C	624	CYS
2	C	630	CYS
2	C	682	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	GLN
1	A	457	ASN
1	A	657	ASN
1	A	1135	ASN
1	A	1153	ASN
1	A	1241	ASN
1	A	1597	GLN
1	A	1971	GLN
1	A	2199	ASN
1	A	2203	HIS
1	A	2307	GLN
1	A	2432	HIS
1	A	2480	ASN
1	A	2496	ASN
1	A	2591	HIS
1	B	73	GLN
1	B	713	GLN
1	B	787	HIS
1	B	827	ASN
1	B	1137	GLN
1	B	1414	GLN
1	B	1542	GLN
1	B	1575	GLN
1	B	1862	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1926	GLN
1	B	2056	ASN
1	B	2131	ASN
1	B	2382	ASN
1	B	2480	ASN
1	B	2517	HIS
2	D	303	GLN
2	D	387	ASN
2	D	424	GLN
2	D	535	GLN
2	D	574	ASN
2	D	657	GLN
2	C	306	ASN
2	C	584	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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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
3	A1EIK	B	2701	-	31,35,35	0.80	1 (3%)	33,53,53	1.51	4 (12%)
3	A1EIK	A	2701	-	31,35,35	0.71	0	33,53,53	1.14	5 (15%)

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
3	A1EIK	B	2701	-	-	2/10/44/44	0/7/6/6
3	A1EIK	A	2701	-	-	4/10/44/44	0/7/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2701	A1EIK	C15-N14	-2.25	1.40	1.44

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2701	A1EIK	O4-C3-C2	-5.84	94.99	111.48
3	A	2701	A1EIK	C21-C20-C11	-3.56	116.14	119.98
3	B	2701	A1EIK	C21-C20-C11	-3.25	116.47	119.98
3	B	2701	A1EIK	C8-N9-C10	-2.71	114.74	118.75
3	A	2701	A1EIK	C8-N9-C10	-2.48	115.09	118.75
3	A	2701	A1EIK	C6-N7-C8	2.35	125.85	120.40
3	A	2701	A1EIK	O4-C3-C2	-2.25	105.13	111.48
3	A	2701	A1EIK	C16-C15-N19	-2.03	107.81	110.55
3	B	2701	A1EIK	C16-C15-N19	-2.00	107.84	110.55

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2701	A1EIK	C21-C8-N7-C2
3	A	2701	A1EIK	N9-C8-N7-C2
3	A	2701	A1EIK	N9-C8-N7-C6
3	A	2701	A1EIK	C21-C8-N7-C6
3	B	2701	A1EIK	C21-C8-N7-C2
3	B	2701	A1EIK	N9-C8-N7-C2

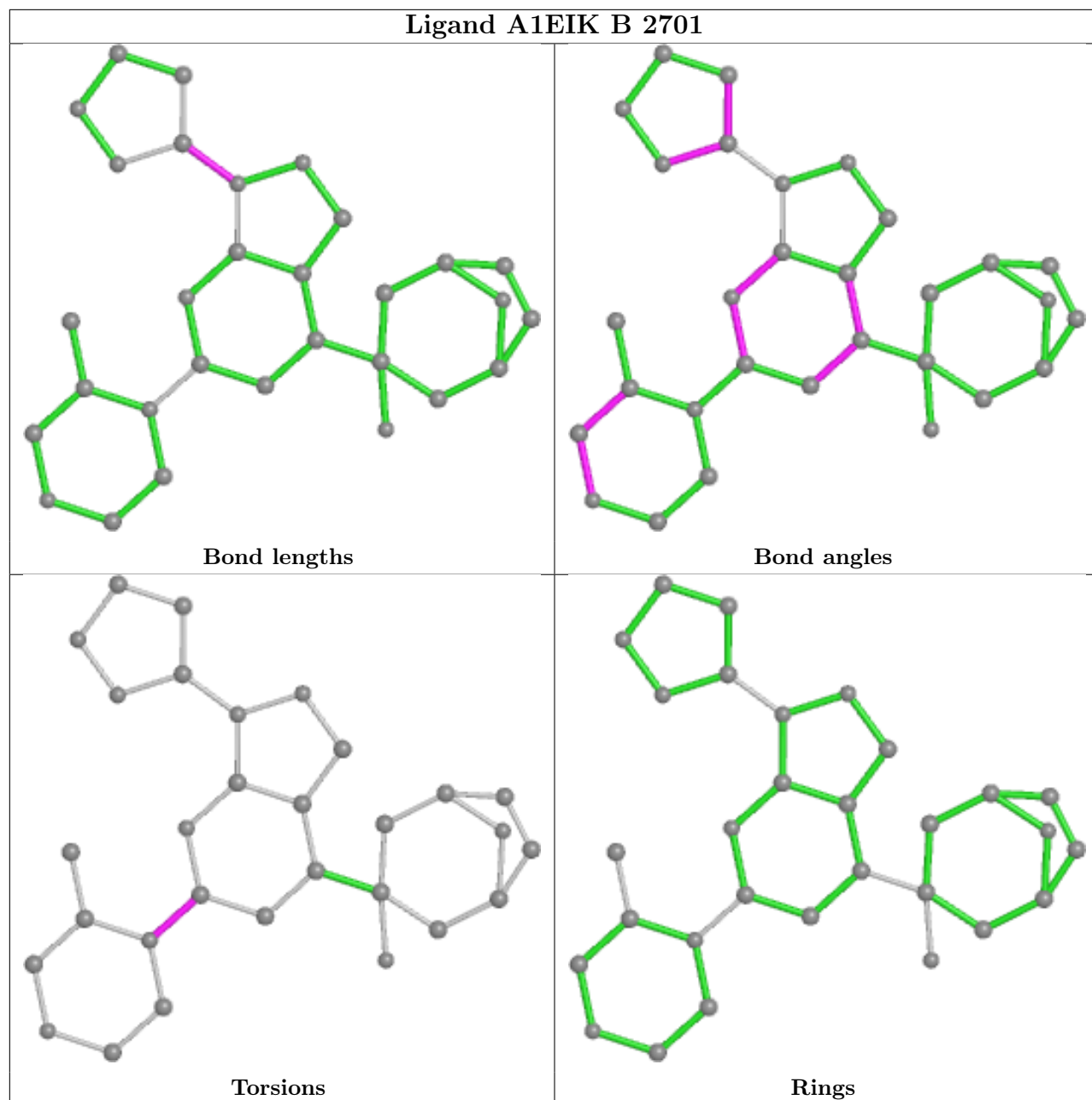
There are no ring outliers.

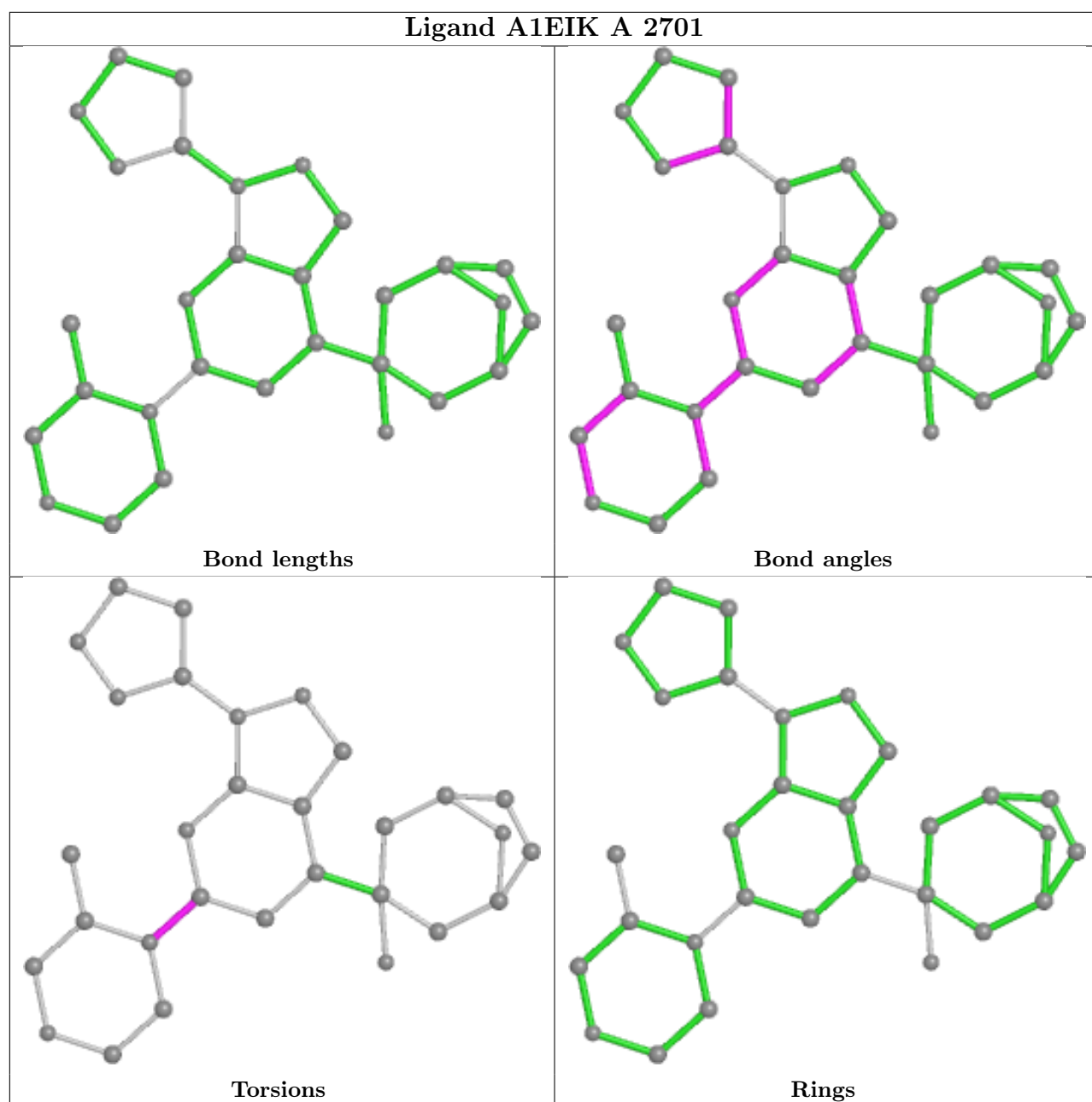
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2701	A1EIK	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand A1EIK B 2701





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.