



## Full wwPDB EM Validation Report ⓘ

Dec 22, 2024 – 12:07 AM JST

PDB ID : 8ZWA  
EMDB ID : EMD-60521  
Title : HopBY induced At EDS1-PAD4-ADR1 heterotrimer  
Authors : Xu, W.Y.; Zhang, Y.; Yu, H.; Wan, L.  
Deposited on : 2024-06-13  
Resolution : 3.48 Å (reported)  
Based on initial model : .

This is a Full wwPDB EM 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/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>.

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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 : 4.02b-467  
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) : 2.40

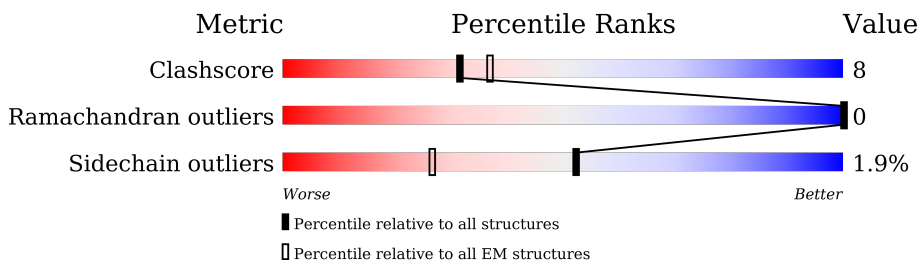
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.48 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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	787	
2	B	623	
3	C	541	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11395 atoms, of which 0 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 Disease resistance protein ADR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	414	2969	1878	504	573	14	0	0

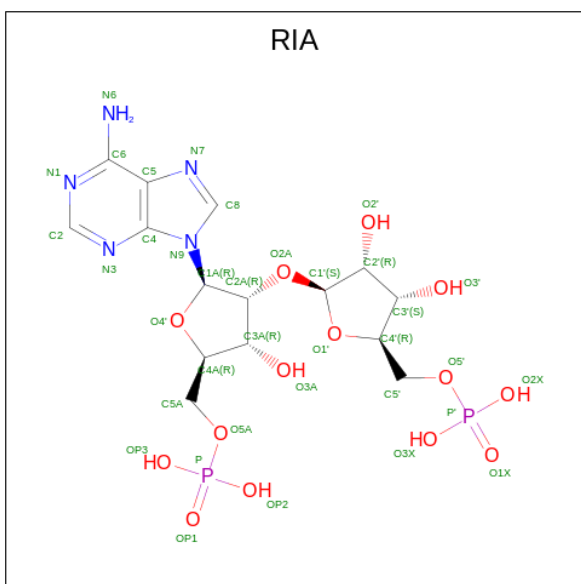
- Molecule 2 is a protein called Isoform 1 of Protein EDS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	577	4416	2805	756	844	11	0	0

- Molecule 3 is a protein called PAD4.

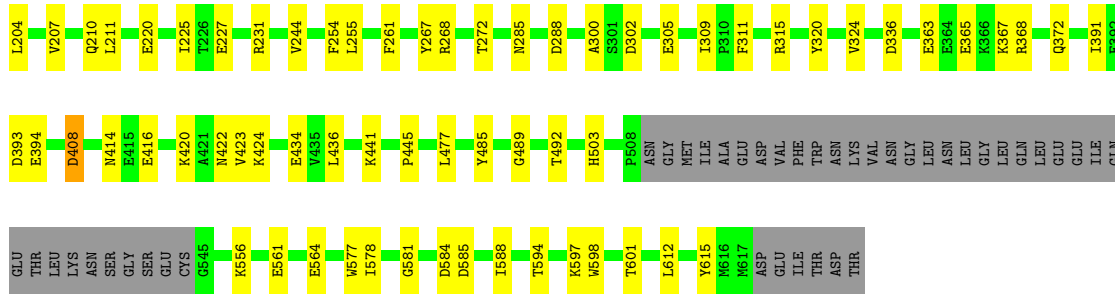
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	518	3974	2524	680	756	14	0	0

- Molecule 4 is 2'-O-[(5'-PHOSPHO)RIBOSYL]ADENOSINE-5'-MONOPHOSPHATE (three-letter code: RIA) (formula:  $C_{15}H_{23}N_5O_{14}P_2$ ).

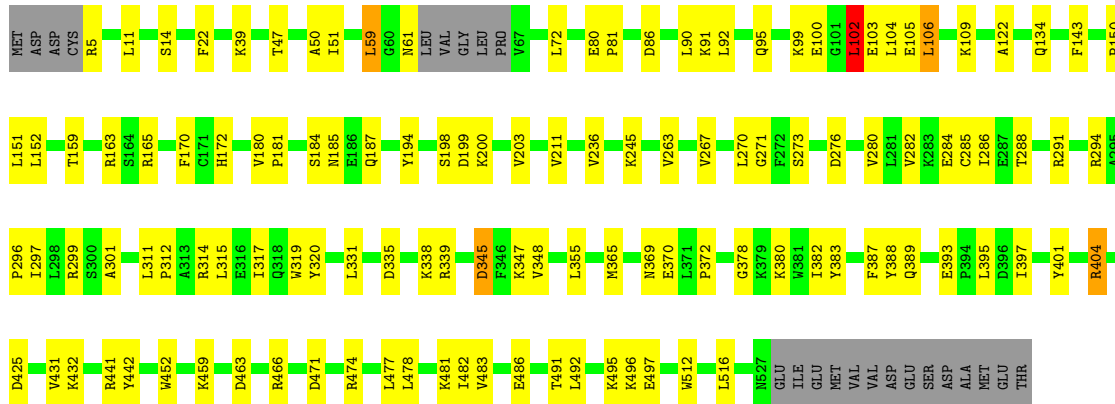


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	B	1	36	15	5	14	2	0





• Molecule 3: PAD4



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	107173	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	55	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k 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: RIA

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	0.45	0/3021	0.53	0/4124
2	B	0.33	0/4514	0.47	0/6122
3	C	0.29	0/4061	0.49	1/5511 (0.0%)
All	All	0.35	0/11596	0.50	1/15757 (0.0%)

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
3	C	0	2
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	102	LEU	CA-CB-CG	5.94	128.96	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	389	ARG	Sidechain
3	C	339	ARG	Sidechain
3	C	5	ARG	Sidechain



## 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	2969	0	2705	68	0
2	B	4416	0	4100	53	0
3	C	3974	0	3777	75	0
4	B	36	0	19	3	0
All	All	11395	0	10601	186	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 8.

All (186) 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:506:LYS:HA	1:A:528:ALA:HA	1.66	0.76
2:B:159:PRO:HA	2:B:190:PRO:HA	1.74	0.69
1:A:481:ARG:H	1:A:507:ILE:HB	1.69	0.58
3:C:299:ARG:HH22	3:C:365:MET:HE1	1.69	0.58
3:C:194:TYR:HD1	3:C:211:VAL:HG11	1.70	0.57
1:A:449:HIS:HB3	1:A:703:TYR:HB2	1.87	0.56
1:A:480:GLU:N	1:A:504:ASP:O	2.38	0.56
1:A:637:HIS:H	1:A:660:ASN:HB2	1.71	0.56
3:C:61:ASN:HB3	3:C:86:ASP:HA	1.88	0.56
2:B:207:VAL:HG12	2:B:225:ILE:HD13	1.87	0.55
1:A:574:ALA:HB1	1:A:596:THR:HA	1.89	0.55
2:B:75:ARG:HB3	2:B:82:VAL:HG12	1.87	0.55
2:B:441:LYS:HG3	3:C:297:ILE:HD12	1.88	0.55
3:C:397:ILE:HD11	3:C:452:TRP:HB2	1.89	0.55
1:A:408:LEU:HD21	1:A:556:VAL:HG21	1.89	0.55
3:C:92:LEU:HA	3:C:95:GLN:HG2	1.89	0.55
3:C:104:LEU:HD12	3:C:105:GLU:HG2	1.89	0.55
1:A:784:TRP:CZ3	3:C:347:LYS:HB3	2.42	0.54
1:A:600:LYS:HA	1:A:628:PRO:HD2	1.88	0.54
3:C:59:LEU:HD12	3:C:152:LEU:HB3	1.89	0.54
2:B:408:ASP:OD2	2:B:594:THR:N	2.40	0.54
1:A:660:ASN:HA	1:A:684:ALA:HB3	1.90	0.54
2:B:285:ASN:ND2	2:B:336:ASP:OD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:273:SER:HB3	3:C:276:ASP:HB2	1.91	0.53
1:A:576:LEU:HG	1:A:578:LYS:H	1.74	0.53
2:B:434:GLU:HG3	3:C:301:ALA:HB1	1.90	0.53
1:A:506:LYS:CA	1:A:528:ALA:HA	2.38	0.53
1:A:664:ILE:HB	1:A:685:CYS:SG	2.49	0.53
2:B:13:LEU:HD11	2:B:38:VAL:HG11	1.90	0.53
2:B:300:ALA:HB3	3:C:245:LYS:HA	1.91	0.53
2:B:612:LEU:HA	2:B:615:TYR:HD2	1.73	0.53
3:C:314:ARG:HA	3:C:317:ILE:HG22	1.91	0.52
3:C:163:ARG:O	3:C:165:ARG:NH1	2.42	0.52
3:C:276:ASP:O	3:C:280:VAL:N	2.37	0.51
2:B:320:TYR:O	2:B:324:VAL:HG23	2.12	0.50
3:C:151:LEU:HD23	3:C:184:SER:HB2	1.93	0.50
3:C:338:LYS:HZ2	3:C:401:TYR:HB3	1.76	0.50
1:A:381:LEU:CD1	1:A:389:ARG:HG3	2.41	0.50
2:B:172:ARG:NH1	2:B:173:GLU:OE2	2.44	0.50
3:C:51:ILE:HD12	3:C:51:ILE:H	1.76	0.50
2:B:261:PHE:CE2	3:C:143:PHE:HB2	2.46	0.50
1:A:674:VAL:HG12	1:A:677:LEU:HB2	1.94	0.50
2:B:391:ILE:HD11	2:B:424:LYS:HB2	1.93	0.50
1:A:416:ARG:HG2	1:A:507:ILE:HD11	1.94	0.50
3:C:72:LEU:O	3:C:134:GLN:NE2	2.44	0.50
1:A:408:LEU:O	1:A:412:VAL:HG12	2.12	0.50
3:C:478:LEU:O	3:C:482:ILE:HG12	2.11	0.49
2:B:9:ILE:HG23	2:B:13:LEU:HD23	1.93	0.49
1:A:616:PHE:CE1	1:A:646:SER:HB2	2.47	0.49
1:A:749:ARG:H	1:A:749:ARG:HD2	1.78	0.49
3:C:39:LYS:HB3	3:C:50:ALA:HB3	1.94	0.49
3:C:159:THR:O	3:C:163:ARG:HG3	2.12	0.49
1:A:403:LYS:HD2	1:A:456:PHE:HB3	1.94	0.49
1:A:749:ARG:HG3	1:A:770:GLU:HB3	1.94	0.49
3:C:99:LYS:O	3:C:102:LEU:HD12	2.12	0.49
3:C:378:GLY:O	3:C:380:LYS:N	2.44	0.48
3:C:370:GLU:N	3:C:370:GLU:OE1	2.46	0.48
1:A:518:MET:HA	1:A:544:PRO:HD2	1.96	0.48
3:C:320:TYR:CD2	3:C:348:VAL:HG21	2.48	0.48
2:B:134:VAL:HG21	2:B:166:PHE:HZ	1.80	0.47
1:A:565:ALA:HB3	1:A:587:VAL:HG22	1.95	0.47
2:B:584:ASP:O	2:B:588:ILE:HG12	2.15	0.47
2:B:489:GLY:HA2	4:B:701:RIA:H8	1.79	0.47
1:A:591:GLU:HA	1:A:615:SER:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:ASP:HB3	1:A:625:LYS:HD3	1.96	0.47
2:B:154:VAL:HA	2:B:180:VAL:O	2.15	0.47
1:A:539:ASN:HA	1:A:566:ARG:HB2	1.97	0.47
3:C:314:ARG:HB2	3:C:355:LEU:HD21	1.98	0.47
3:C:47:THR:HG21	3:C:109:LYS:HE2	1.97	0.46
1:A:460:HIS:HB2	1:A:463:LEU:HG	1.97	0.46
1:A:540:TYR:N	1:A:566:ARG:O	2.48	0.46
1:A:762:GLU:O	1:A:766:LYS:HG2	2.15	0.46
3:C:442:TYR:HA	3:C:496:LYS:HB3	1.96	0.46
2:B:311:PHE:O	2:B:315:ARG:HG2	2.16	0.46
1:A:722:LEU:HG	1:A:725:LEU:HB2	1.97	0.46
2:B:91:LYS:O	2:B:94:GLU:HG2	2.16	0.46
3:C:103:GLU:HA	3:C:106:LEU:HG	1.96	0.46
3:C:122:ALA:HB2	3:C:150:PRO:HD2	1.97	0.46
3:C:312:PRO:HA	3:C:315:LEU:HD12	1.97	0.46
1:A:751:VAL:O	1:A:774:GLU:N	2.43	0.46
2:B:420:LYS:O	2:B:424:LYS:HG2	2.16	0.46
3:C:459:LYS:HG2	3:C:512:TRP:CD1	2.51	0.46
2:B:254:PHE:HD2	2:B:255:LEU:HD22	1.81	0.45
1:A:589:VAL:HG21	1:A:612:VAL:HG23	1.98	0.45
1:A:755:GLU:HA	1:A:775:VAL:HG23	1.97	0.45
2:B:423:VAL:HG22	3:C:312:PRO:HB3	1.98	0.45
3:C:314:ARG:O	3:C:317:ILE:HG22	2.17	0.45
3:C:471:ASP:HB3	3:C:474:ARG:HD3	1.98	0.45
1:A:484:MET:SD	1:A:484:MET:N	2.90	0.45
1:A:698:LEU:HD12	1:A:701:LEU:HD22	1.98	0.45
1:A:745:LEU:HD22	1:A:747:SER:H	1.80	0.45
2:B:49:GLU:HG3	2:B:204:LEU:HD23	1.97	0.45
3:C:288:THR:O	3:C:291:ARG:NH1	2.49	0.45
2:B:393:ASP:OD2	2:B:394:GLU:HG2	2.16	0.45
1:A:443:PRO:HG2	1:A:453:TYR:HB3	1.99	0.45
1:A:762:GLU:HA	1:A:765:LYS:HB3	1.98	0.45
1:A:631:SER:O	1:A:654:ASN:N	2.36	0.45
2:B:74:MET:SD	2:B:74:MET:N	2.90	0.45
3:C:294:ARG:HG2	3:C:299:ARG:HD2	1.99	0.45
3:C:483:VAL:O	3:C:486:GLU:HG3	2.16	0.45
3:C:198:SER:OG	3:C:199:ASP:N	2.50	0.44
3:C:369:ASN:O	3:C:369:ASN:CG	2.55	0.44
2:B:363:GLU:O	2:B:367:LYS:HG2	2.16	0.44
2:B:414:ASN:HA	3:C:319:TRP:CH2	2.53	0.44
3:C:185:ASN:HB3	3:C:187:GLN:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:SER:HA	1:A:749:ARG:NE	2.32	0.44
3:C:90:LEU:HD12	3:C:91:LYS:N	2.32	0.44
3:C:382:ILE:HG21	3:C:431:VAL:HG12	2.00	0.44
1:A:749:ARG:HA	1:A:770:GLU:O	2.18	0.44
3:C:492:LEU:HG	3:C:497:GLU:HB2	2.00	0.44
1:A:602:LEU:O	1:A:629:SER:HA	2.18	0.44
1:A:754:ASP:HA	1:A:776:ALA:HB3	2.00	0.44
1:A:391:CYS:HB3	1:A:413:TRP:CD2	2.53	0.44
1:A:580:ARG:HA	1:A:602:LEU:HA	1.99	0.44
2:B:118:VAL:HG22	2:B:152:ARG:HB2	1.99	0.44
2:B:577:TRP:O	2:B:581:GLY:N	2.41	0.44
3:C:393:GLU:O	3:C:397:ILE:HG23	2.17	0.44
1:A:413:TRP:HB3	1:A:419:ILE:HD11	1.99	0.43
1:A:414:VAL:HG22	1:A:419:ILE:O	2.18	0.43
4:B:701:RIA:H4A	3:C:380:LYS:HG3	2.00	0.43
3:C:172:HIS:HB3	3:C:194:TYR:CD2	2.52	0.43
1:A:538:ASP:OD1	1:A:539:ASN:N	2.50	0.43
1:A:391:CYS:HB3	1:A:413:TRP:CE2	2.53	0.43
2:B:597:LYS:O	2:B:601:THR:HG23	2.18	0.43
1:A:622:ASP:O	1:A:626:ILE:HG12	2.17	0.43
2:B:365:GLU:OE1	2:B:368:ARG:NH1	2.51	0.43
3:C:355:LEU:HD23	3:C:388:TYR:HD1	1.81	0.43
3:C:463:ASP:HA	3:C:466:ARG:NE	2.34	0.43
3:C:491:THR:O	3:C:495:LYS:HG2	2.18	0.43
1:A:564:PRO:HB2	1:A:588:HIS:NE2	2.34	0.43
1:A:381:LEU:HD11	1:A:389:ARG:HG3	2.01	0.43
1:A:449:HIS:HB3	1:A:703:TYR:CB	2.48	0.43
2:B:207:VAL:O	2:B:211:LEU:HD23	2.19	0.43
3:C:280:VAL:O	3:C:284:GLU:HG2	2.18	0.43
2:B:96:ILE:O	2:B:101:THR:OG1	2.31	0.43
3:C:203:VAL:HG21	3:C:270:LEU:HD23	2.00	0.43
2:B:556:LYS:NZ	2:B:598:TRP:HB2	2.34	0.43
2:B:578:ILE:HG21	2:B:585:ASP:HB3	2.01	0.43
1:A:653:LEU:HD23	1:A:674:VAL:HG11	2.00	0.43
2:B:73:CYS:HB3	2:B:503:HIS:HE1	1.84	0.43
1:A:734:SER:O	1:A:736:LEU:HG	2.18	0.42
1:A:404:ILE:HD12	1:A:405:PRO:HD2	2.01	0.42
2:B:227:GLU:O	2:B:231:ARG:HG2	2.19	0.42
3:C:22:PHE:CE2	3:C:236:VAL:HG23	2.55	0.42
3:C:200:LYS:HD2	3:C:271:GLY:HA2	2.02	0.42
3:C:317:ILE:HD11	3:C:395:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:GLU:O	3:C:81:PRO:C	2.56	0.42
2:B:71:PHE:HB3	2:B:74:MET:HG2	2.01	0.42
2:B:477:LEU:HD11	3:C:441:ARG:HH21	1.85	0.42
2:B:267:TYR:O	2:B:268:ARG:HD3	2.20	0.42
3:C:389:GLN:NE2	3:C:425:ASP:OD1	2.38	0.42
1:A:751:VAL:HG23	1:A:771:LEU:O	2.20	0.41
2:B:556:LYS:HE2	2:B:556:LYS:HB2	1.89	0.41
3:C:100:GLU:O	3:C:104:LEU:HG	2.20	0.41
2:B:244:VAL:HG13	3:C:11:LEU:HD21	2.02	0.41
3:C:331:LEU:HG	3:C:335:ASP:HB2	2.02	0.41
2:B:561:GLU:O	2:B:564:GLU:HG3	2.20	0.41
3:C:263:VAL:O	3:C:267:VAL:HG23	2.20	0.41
1:A:656:LEU:HD21	1:A:658:ILE:HD11	2.01	0.41
2:B:92:ASN:O	2:B:96:ILE:HG12	2.21	0.41
3:C:431:VAL:HG23	3:C:432:LYS:O	2.19	0.41
1:A:506:LYS:HA	1:A:529:GLU:H	1.85	0.41
2:B:177:ARG:HH21	2:B:272:THR:HG1	1.68	0.41
1:A:627:PHE:C	1:A:629:SER:H	2.23	0.41
2:B:305:GLU:CB	2:B:309:ILE:HD11	2.51	0.41
3:C:263:VAL:HG22	3:C:286:ILE:HG22	2.02	0.41
3:C:296:PRO:HB2	3:C:372:PRO:HD3	2.02	0.41
1:A:505:ALA:O	1:A:508:VAL:HG23	2.21	0.41
2:B:58:LYS:HE2	2:B:58:LYS:HB2	1.90	0.41
2:B:210:GLN:NE2	2:B:220:GLU:HA	2.36	0.41
3:C:282:VAL:HA	3:C:285:CYS:SG	2.60	0.41
1:A:406:LEU:O	1:A:410:THR:HG22	2.21	0.41
3:C:180:VAL:HB	3:C:181:PRO:HD3	2.01	0.41
1:A:565:ALA:O	1:A:588:HIS:N	2.40	0.41
1:A:723:GLY:HA2	1:A:745:LEU:CD2	2.51	0.41
4:B:701:RIA:N3	3:C:383:TYR:HB3	2.36	0.41
3:C:311:LEU:CD1	3:C:314:ARG:HE	2.34	0.41
3:C:477:LEU:O	3:C:481:LYS:HG3	2.21	0.41
1:A:432:ALA:HA	1:A:437:LEU:HD22	2.03	0.40
1:A:683:TYR:O	1:A:708:GLN:HB2	2.21	0.40
1:A:782:VAL:HG22	2:B:416:GLU:HG2	2.02	0.40
3:C:401:TYR:HD1	3:C:404:ARG:HD2	1.85	0.40
3:C:345:ASP:O	3:C:348:VAL:HG12	2.21	0.40
2:B:372:GLN:HB2	2:B:445:PRO:CD	2.50	0.40
2:B:436:LEU:HD21	2:B:492:THR:OG1	2.22	0.40
1:A:714:SER:H	1:A:736:LEU:H	1.69	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	412/787 (52%)	391 (95%)	21 (5%)	0	100	100
2	B	571/623 (92%)	565 (99%)	6 (1%)	0	100	100
3	C	514/541 (95%)	504 (98%)	10 (2%)	0	100	100
All	All	1497/1951 (77%)	1460 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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 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	293/729 (40%)	287 (98%)	6 (2%)	50	72
2	B	440/548 (80%)	433 (98%)	7 (2%)	58	76
3	C	410/474 (86%)	401 (98%)	9 (2%)	47	70
All	All	1143/1751 (65%)	1121 (98%)	22 (2%)	52	73

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	385	ASP
1	A	583	TRP
1	A	681	ARG
1	A	683	TYR
1	A	745	LEU

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	784	TRP
2	B	148	TYR
2	B	149	LEU
2	B	288	ASP
2	B	302	ASP
2	B	408	ASP
2	B	422	ASN
2	B	485	TYR
3	C	14	SER
3	C	59	LEU
3	C	102	LEU
3	C	106	LEU
3	C	170	PHE
3	C	345	ASP
3	C	387	PHE
3	C	404	ARG
3	C	516	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	70	GLN
2	B	414	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

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
4	RIA	B	701	-	35,39,39	3.36	11 (31%)	46,60,60	1.19	3 (6%)

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
4	RIA	B	701	-	-	4/16/52/52	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	701	RIA	O4'-C1A	-9.20	1.28	1.41
4	B	701	RIA	O1'-C1'	8.75	1.57	1.41
4	B	701	RIA	C3'-C4'	-8.63	1.30	1.53
4	B	701	RIA	O1'-C4'	5.57	1.57	1.45
4	B	701	RIA	O3A-C3A	4.70	1.54	1.43
4	B	701	RIA	C3'-C2'	4.54	1.65	1.53
4	B	701	RIA	C6-N6	4.08	1.48	1.34
4	B	701	RIA	O4'-C4A	3.67	1.53	1.45
4	B	701	RIA	C5A-C4A	-2.93	1.42	1.51
4	B	701	RIA	P'-O5'	2.61	1.68	1.60
4	B	701	RIA	C1'-C2'	-2.18	1.50	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	RIA	N3-C2-N1	-4.38	121.83	128.68
4	B	701	RIA	C1'-O2A-C2A	-3.58	109.11	117.96
4	B	701	RIA	C4-C5-N7	-2.23	107.08	109.40

There are no chirality outliers.



All (4) torsion outliers are listed below:

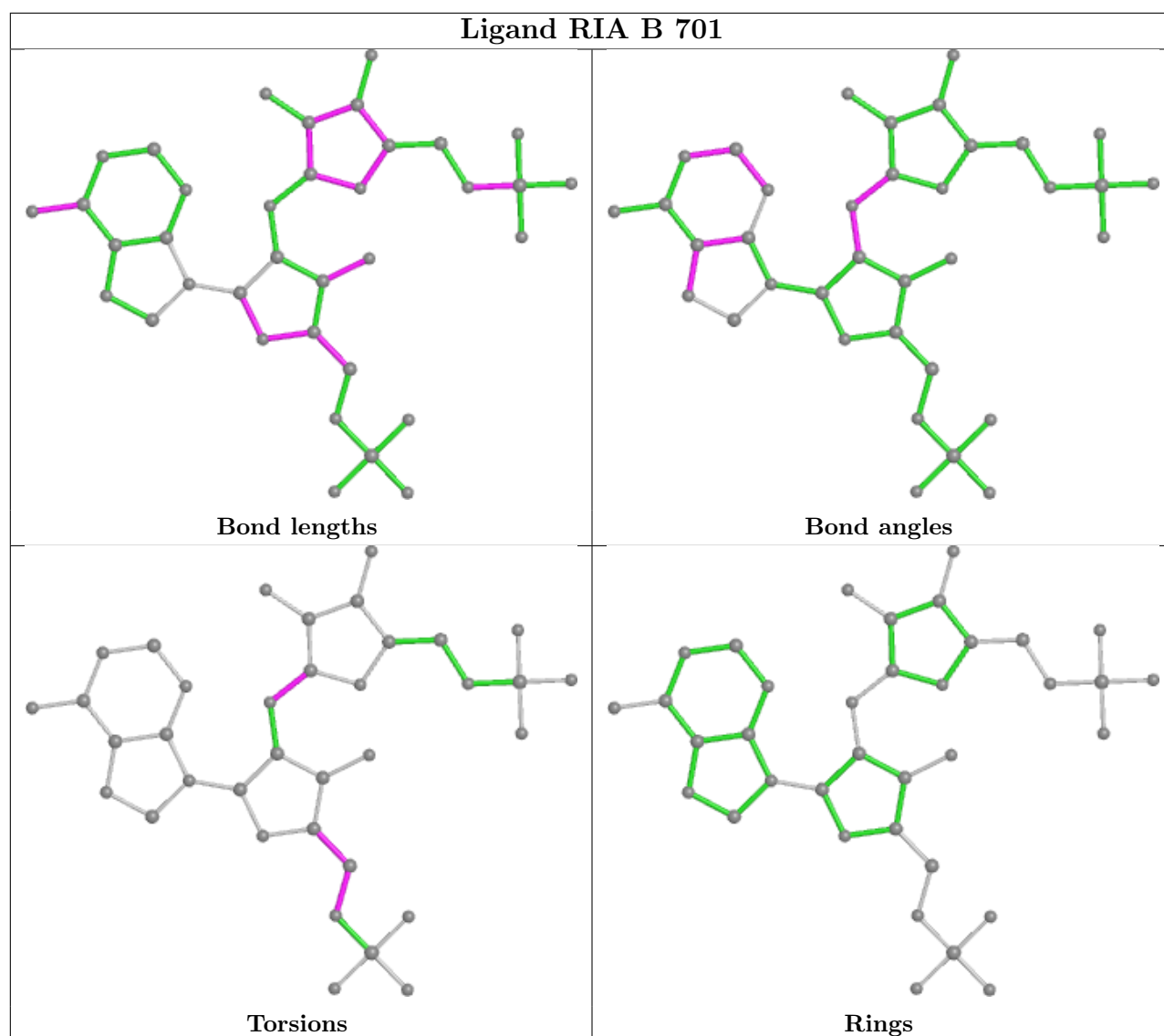
Mol	Chain	Res	Type	Atoms
4	B	701	RIA	O4'-C4A-C5A-O5A
4	B	701	RIA	O1'-C1'-O2A-C2A
4	B	701	RIA	C4A-C5A-O5A-P
4	B	701	RIA	C2'-C1'-O2A-C2A

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	701	RIA	3	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.